

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

FCIC Task 4 – Data Integration and Web Portal Development

April 6, 2023

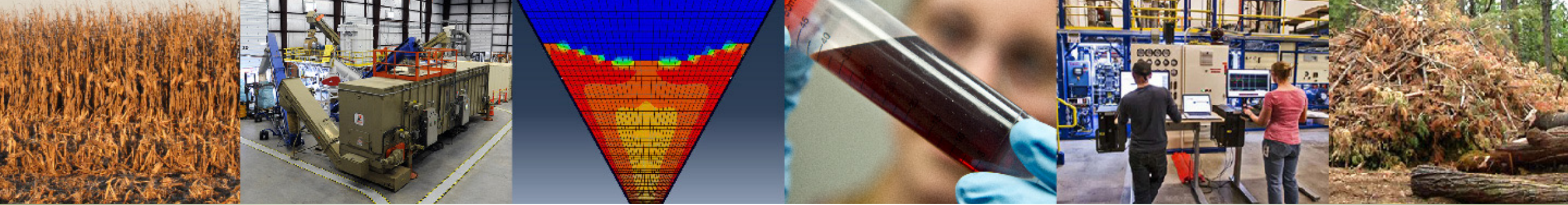
Feedstock-Conversion Interface Consortium (FCIC)

Jim Collett – PNNL

Rachel Emerson - INL

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Project Overview



FCIC Task Organization

Feedstock **Preprocessing** **Conversion**

Task 2: Feedstock Variability

Task 5: Preprocessing

Task 6: High-Temperature Conversion

Task 1: Materials of Construction

Task 7: Low-Temperature Conversion

Task 3: Materials Handling

Enabling Tasks

Task X: Project Management

Task 4: Data Integration

Task 8: TEA/LCA
Task 9: FMEA

Task X: Project Management: Provide scientific leadership and organizational project management

Task 1: Materials of Construction: Specify materials that do not wear, or break at unacceptable rates

Task 2: Feedstock Variability: Quantify & understand the sources of biomass resource and feedstock variability

Task 3: Materials Handling: Develop tools that enable continuous, steady, trouble free feed into reactors

Task 4: Data Integration: Ensure the data generated in the FCIC are curated and stored – FAIR guidelines

Task 5: Preprocessing: Enable well-defined and homogeneous feedstock from variable biomass resources

Task 6 & 7: Conversion (High- & Low-Temp Pathways): Produce intermediates for further processing

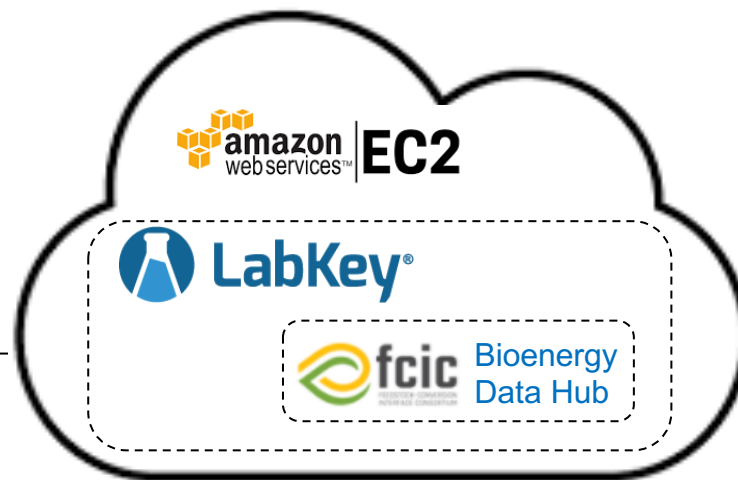
Task 8: Crosscutting Analyses TEA/LCA: Valuation of intermediate streams & quantify variability impact

Task 9: Failure Mode & Effects Analysis (FMEA): Standardized approach for assessing attribute criticality



Task 4 Project Overview

- **Objective:** To provide a web-enabled database and public web portal for integrating, standardizing, and distributing FCIC data to industry stakeholders.
- **Impact:** This Task will accelerate the design and deployment of biorefineries and support their profitable operation by providing a “one-stop shop” for up-to-date data and information on understanding and mitigating the impacts of feedstock variability on bioenergy conversion processes.
- **Outcome:** An online community of industry and DOE stakeholders sharing data, knowledge, and tools via the FCIC Bioenergy Data Hub with a target of having 100+ active users from commercial entities.



Industry Stakeholders



Feedstock Producers



Equipment Designers



Biorefinery Integrators



R&D Teams



The Task 4 Team



Jim Collett
PNNL
Task Lead
Site Architecture;
Data Tool
Integration;
Task & Subtask
Content; Planning
and Budgeting;
Low Temperature
Conversion SME*



Rachel Emerson
INL
Task Co-Lead
Site Architecture;
Case Study Web
Design &
Publishing; FMEA**
Integration;
Interface to
Bioenergy
Feedstock Library;
Feedstocks SME



Bob Kinoshita
INL
Data Tool Design;
JavaScript, Python,
and R Coding;
Preprocessing SME



Anne Starace
NREL
Case Study Web
Design &
Publishing; High
Temperature
Conversion SME



Shaun O'Leary
PNNL
AWS*** Cloud
Infrastructure; Site
Security; DOE
Policy Compliance



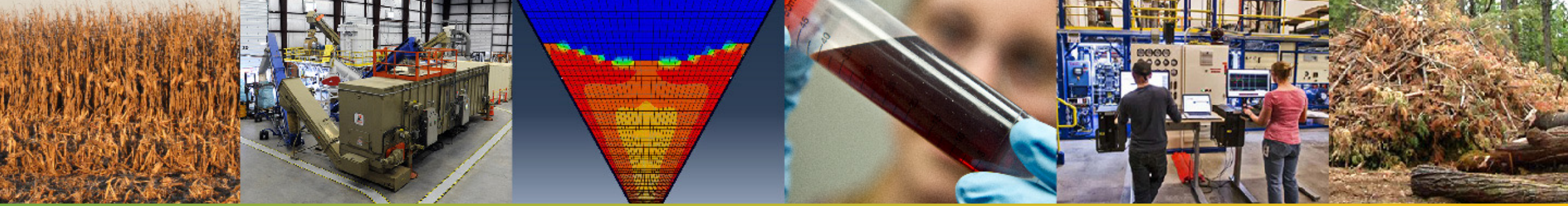
Matt Macduff
PNNL
LabKey Server
and Database
Administration

*Subject Matter Expert

**Failure Mode Effects Analysis



***Amazon Web Services



1 – Approach

1 – Approach

The Data Integration and Web Portal Task targets FY21 Peer Review recommendations to:


- Develop innovative ways to immerse the national laboratories with industry.
- Establish quality specifications on feedstocks
- Aggressively promote FCIC results and visibility

bioenergy.labworks.org/labkey/FCIC/project-begin.view

fcic Bioenergy Data Hub

FCIC Knowledge & Tools by Task Case Studies Home Page Task Teams & Publications Biorefinery Designs Quality by Design

Welcome to the **Feedstock-Conversion Interface Consortium (FCIC)** Data Hub



Argonne **Berkeley Lab** **INL**
Los Alamos **NREL** **Oak Ridge**
Pacific Northwest **Sandia**

The **FCIC** is a collaborative effort among researchers from nine National Laboratories that is sponsored by the U.S. Department of Energy's **Bioenergy Technologies Office (BETO)**.

The mission of the FCIC is to develop knowledge and tools to understand and mitigate the effects feedstock and process variability on biorefinery performance. The consortium is organized into eight complementary Task areas:

(1) **Materials of Construction**; (2) **Feedstock Variability**; (3) **Materials Handling**; (4) **Data Integration and Web Portal Development**; (5) **Feedstock Preprocessing**; (6) **High Temperature Conversion**; (7) **Low Temperature Conversion**; (8) **Crosscutting Analyses with Systematic Criticality Assessment**.

The **R&D Teams & Publications** tab at the top of this page provides links to information, data, tools, and publications produced by Subtask Study teams within each of the FCIC Tasks. You can view the FCIC's current lists of Critical Properties for biorefinery unit operations and for feedstock, intermediate, and product streams under the **Biorefinery Designs** tab.

2022 Annual Meeting Posters

PDF
000-FCIC FY22 Annual Poster Session Abstracts.pdf
001-Appling advanced blade materials.pdf
002-Characterizing Biomass Feedstock Transport Properties Using State of the Art Imaging and Computational Techniques.pdf
003-Drought impact on anatomical fractions of corn stover as bioenergy feedstock.pdf
004-Effect of Moisture and Feedstock Variability on the rheological Behavior of Corn Stover.pdf
005-Corn Stalk Knife Milling Model.pdf
006-LowT Conversion_Experimentally Trained Models.pdf

For technical assistance, please contact:
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Rachel Emerson rachel.emerson@inl.gov 208-526-1931

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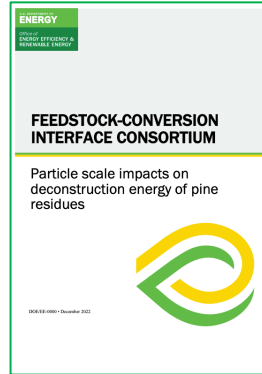
The **FCIC Bioenergy Data Hub** is now online for invited user testing at <https://bioenergy.labworks.org/labkey/FCIC>



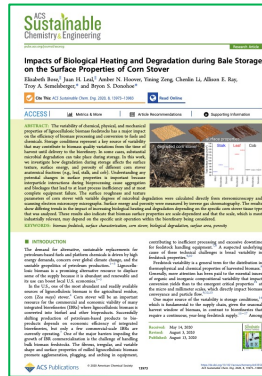
1 – Approach



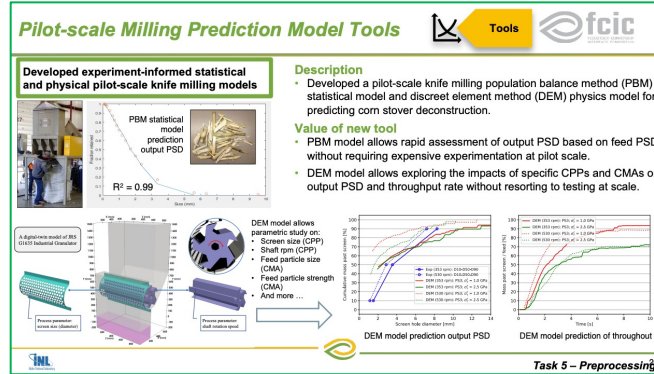
- Task 1. Materials of Construction
- Task 2. Feedstock Variability
- Task 3. Materials Handling
- Task 5. Feedstock Preprocessing
- Task 6. High-Temperature Conversion
- Task 7. Low Temperature Conversion
- Task 8. Cross-Cutting Analysis and Systemic Criticality Assessment
- Task 9. Failure Mode & Effects Analysis (FMEA):



FCIC Case Studies (5)



Journal Articles (78)



Knowledge and Tool Slides (135)

fcic Bioenergy Data Hub

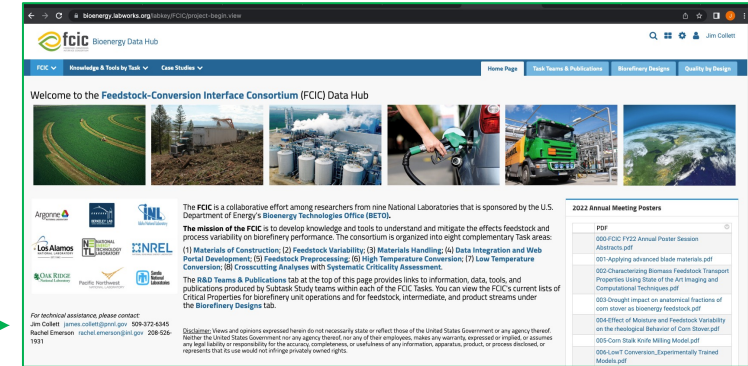
Sensitivity analysis of air classification of forest residue for tissue and ash separation efficiency (HT-P-11_02)

The data below are the results from the case study TEA analysis. See full data sets in the here under the Datasets and Lists webpages.

Design ID	Technology Pathway	MFSP Mean (\$/GGE)	Mean Delivered Feedstock Cost (\$/dry ton)	Added Cost of Quality Disposal (\$/dry ton)	Overall Operating Effectiveness (OEE, %)	Quality Performance Factor (F _{BP})	Total Production Cost Mean (\$/dry ton)	Added Cost of Lost Material (\$/dry ton)
HT-P-11_BC_0Hz_0.6mm_18FC	11_BaseCase	4.78	621.82	\$30.36	12.02	0.15	91.46	16.69
HT-P-11_BC_0Hz_0.6mm_21FC	11_BaseCase	4.76	123.58	32.13	60.49	0.75	91.45	16.70
HT-P-11_BC_0Hz_0.7mm_18FC	11_BaseCase	5.06	713.8	608.81	10.47	0.15	105.00	30.26
HT-P-11_BC_0Hz_0.7mm_21FC	11_BaseCase	5.07	142.2	36.96	52.68	0.75	105.25	30.34
HT-P-11_BC_0Hz_1.18mm_18FC	11_BaseCase	5.77	931.32	794.19	8.01	0.15	137.14	62.53
HT-P-11_BC_0Hz_1.18mm_21FC	11_BaseCase	5.78	186.02	48.36	40.29	0.75	137.66	62.77

Supporting Datasets

Task 4. Data Integration & Web Portal Development

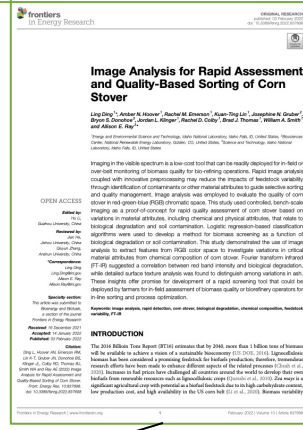
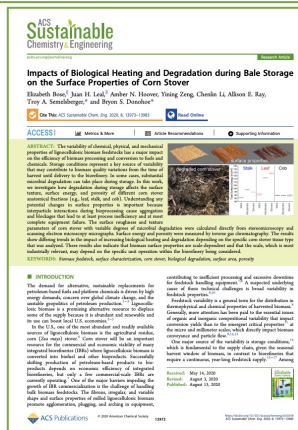
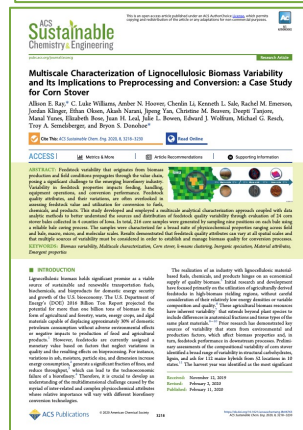


The **FCIC Bioenergy Data Hub** provides industry stakeholders with integrated access to Case Studies, Journal Articles, Knowledge and Tool Slides and Technical Reports produced by FCIC Researchers from 9 National Labs (NLs) who collaborate within 34 subtask teams within 8 experimental and analytical tasks.



1 – Approach

Data integration and enhancement across publications to increase their value to stakeholders

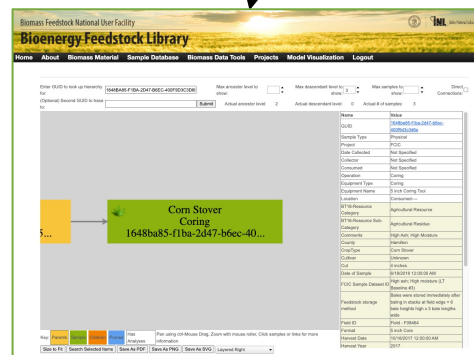
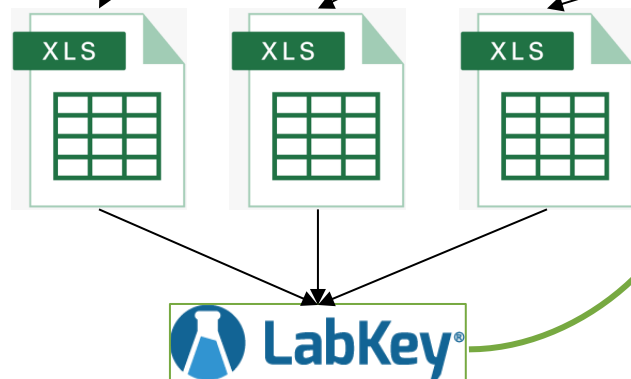


fcic Bioenergy Data Hub

FCIC Task Portals Studies Overview Results Datasets Data Views Workbooks Samples Files Manage

Dataset: Images RGB Experiments

Sample ID	Date	BFL GUID	Image ID, rep1	Image, rep1	ImageID, rep2	Image, rep2	ImageID, rep3	Image, rep3	Reference Image
HMHA_Bale1001_Core10	2018-09-19	1648BA85-F1BA-2D47-B6EC-400F9D3C3D6E	P1060127.JPG	P1060127.jpg					
HMHA_Bale1001_Core11	2018-09-19	C6CDB828-00CF-BA4A-BCD7-5884474719241	P1060115.JPG						
HMHA_Bale1001_Core12	2018-09-19	A2B285BB-857E-344F-9FDE-4423BEFAFFAC	P1060123.JPG						
HMHA_Bale1021_Core10	2018-09-19	544ED4B9-404F-A848-BE48-1EE6367B3460	P1060107.JPG	P1060108.JPG	P1060109.JPG				



LabKey dataset showing image data used within Subtask 2.4. “BFL GUID” column entries directly link to samples in the Bioenergy Feedstock Library at INL.

Image Analysis for Rapid Assessment and Quality-Based Sorting of Corn Stover. Ling, et al. FRONTIERS IN ENERGY RESEARCH, 2022.
<https://doi.org/10.3389/fenrg.2022.837698>

1 – Approach

Technical Approach

- Deploy the FCIC Bioenergy Data Hub using the open source [LabKey web application platform](#) to make FCIC data and information **F**indable, **A**ccessible, **I**nteroperable, and **R**eusable (FAIR) in accordance with the DOE Office of Science and Technology Information's [Research Data Management Policy](#).

Challenges

- Incentivizing our R&D teams to [use the FCIC-branded Data Hub as a “one-stop-shop”](#) for connecting with stakeholders to resolve feedstock-conversion interface challenges. We have met this challenge by [finding and supporting Data Hub champions](#) at each of the member National Labs.
- [Harmonizing data terms and units of measure](#) across FCIC Case Studies to create value for stakeholders who now must parse such information from a variety of journals, NL technical reports, and PowerPoint files on the Internet.

Metrics

- Technical: [User Activity Tracking](#): numbers of Data Hub site visitors once Data Hub is fully public; variety and quantity of FCIC information products on the site; number of log-ons to view/download new FCIC knowledge products when they are promoted via email or other channels.
- Impact: [Focus groups and surveys](#) at conferences, on the Data Hub itself, and emailed directly to stakeholders.

Risks/Mitigation Strategies

- [Sustained commitment from FCIC Leadership](#) to support common data standards and to encourage timely data uploading, integration, and dissemination are essential for engendering stakeholder confidence in the FCIC.
- [Meeting User Experience expectations](#) and maintaining near 100% uptime are necessary to turn new Data Hub users into devoted fans of FCIC knowledge products and tools.



Risks/Mitigation Strategies (continued)

- LabKey Premium Edition Server Software on the FCIC Data Hub provides [enterprise-grade, commercial-quality web application software](#) deployed on the [Amazon Web Services cloud](#) for excellent uptime and availability with same-day technical support and weekly meetings with LabKey software engineers.
- Datasets and code are compatible with the free, open-source Community Edition of LabKey Server to allow [legacy access to data and information](#) if funding for the consortium is discontinued.
- [Separate “production” and “development” servers](#) are maintained by a professional IT team at PNNL to minimize risks of code deployment and software upgrades.

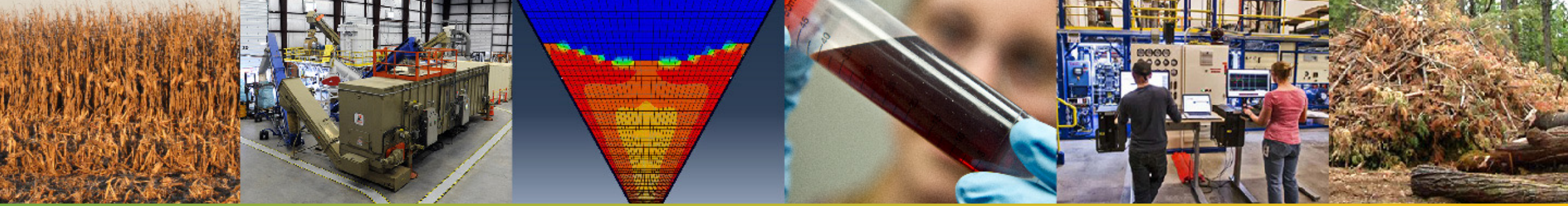
Communication/Collaboration

- Two Task 4 Team meetings per month; [Collaboration between Task 4 Team and experimental and analytical task teams](#) to standardize data terms and units of measure and to development web content for Case Studies hosted on the Data Hub.

DEI

- The LabKey platform has been successfully used to [support DEI outreach](#) to high school science classes in other BETO-funded work (2.3.4.106) and may be leveraged within the FCIC to support DEI within Task X.





2 – *Progress and Outcomes*

2 – Progress – FCIC Data Stakeholder Advisory Panel provided guidance on Data Hub Design and Content

- **Brandon Emme**, FCIC IAB, Head of Engineering and Operations, Technology Development at ICM, Inc.
- **Glenn Farris**, FCIC IAB, Executive Vice President Of Operations at Lee Enterprises Consulting, Inc.
- **Mel Koch**, Principal Scientist, Assoc. Dir., UW Center for Process Analysis and Control; former Global Director of Analytical Services at Dow
- **Ray Chrisman**, Principal, Chrisman Consulting; Affiliate Faculty, UW Forest Resources; former Technology Manager at Dow
- **Mark Penshorn**, Lead Chemical Engineer at ICF; 2021 FCIC Peer Review Panel Lead
- **Steve Hanson**, Account Manager, Director of User Education, LabKey Software
- **Adam Rauch**, Vice President of Product Strategy, LabKey Software

Data Hub is now open to non-DOE users on a limited basis for beta testing. Full opening planned for FY23.

Topics Considered

- FCIC Data Integration and Sharing
 - Data Hub Overall Design
 - Task/Subtask Teams & Workflow Vision
 - Data Finder
 - Quality by Design for Biorefineries
 - Case Studies
 - Building a community of bioeconomy stakeholders

Feedback Summary

- **Users will be interested in specific questions** (such as ash content before and after a given unit operation)
- Suggested integration of data beyond FCIC studies
- Make strong connection to BFL and Phyllis2
- Ensure clear navigation, help, and tutorials
- Analytical methods behind data essential
- Data Hub is a great way to get to know the researchers behind FCIC work



2 – Progress – New Case Study Content and Redesign for Integrated Data Access

Task 4 worked with Task 8 and FCIC leadership to harmonize Case Study data and redesign them for **integrated access** on the Data Hub:

- Biomass Deconstruction and Fermentation Performance based on Isolated Anatomical Fractions (LT-C-5)
- Corn stover storage options considering variable degradation within bale stacks (LT-S-1)
- Effect of Tree Age and Fraction on Fast Pyrolysis (HT-C-7)
- Particle scale impacts on deconstruction energy (HT-P-5).
- Sensitivity analysis of air classification of forest residue for tissue and ash separation efficiency (HT-P-11_02)

Case Study 1: Corn stover storage options considering variable degradation within bale stacks (LT-S-1)

Executive Summary

This techno-economic analysis case study assesses corn stover storage options considering variable degradation within bale stacks. Prior studies using average estimates of losses and compositional changes during storage miss the operational impacts of biomass variability. This new corn stover techno-economic analysis model better represents moisture migration through biomass bale stacks that create zones of varying degradation, which behave differently in preprocessing and conversion operations. Using this approach, researchers can more accurately estimate costs of storage losses and protected storage, as well as predict the impact of bale-to-bale variability on biorefinery operations.

Results: Moisture migration through biomass bale stacks creates zones of varying degradation that behave differently in preprocessing and conversion operations. In this study, Feedstock-Conversion Interface Consortium (FCIC) researchers developed a mathematical model of degradation zones within a corn stover bale stack based on moisture migration over the course of one year. This allows researchers to more accurately predict the variability of incoming feedstock streams due to changes during storage. Cost reductions in preprocessing or conversion of approximately \$1–\$2/dry ton for tarped stover or \$10/dry ton for covered storage would be necessary to justify the higher investment in storage protection.

Download Full Report **Download 2 Page Summary Report**

Old Approach
Assumes average quality parameters and average dry matter loss.

New Approach
Categorize fractions of delivered biomass by degradation levels.

TEA Results

Design ID	Design condition	Cost (\$/dry ton)
LT-S-1_COVERED_LowMoisture	Low Ambient Moisture (0-20%)	82
LT-S-1_TARPED_HighMoisture	High Ambient Moisture (>20%)	73-74
LT-S-1_TARPED_LowMoisture	Low Ambient Moisture (0-20%)	72-73
LT-S-1_UNCOVERED_HighMoisture	High Ambient Moisture (>20%)	72-74
LT-S-1_UNCOVERED_LowMoisture	Low Ambient Moisture (0-20%)	70-73

Quality by Design — Identified Critical Attributes

Critical Material Attributes (CMAs)	Critical Process Parameters (CPPs)	Critical Quality Attributes (CQAs)
Property Bale Density Bale Size Moisture Content	Property Storage Type	Property Degradation Level

Updated 2022-03-01

Key Information

Study ID for Internal Tracking: T.08.CS.LT-S-1

Management Details

Label	Investigator	Species	POC1	POC2	Information Release Authorization Codes
Case Study 1: Corn stover storage options considering variable degradation within bale stacks (LT-S-1)	Erin Webb, Robin Clark	Corn Stover	Erin Webb	steven phillips	

Participating Organizations

Participating Organizations	Name
INL	Idaho National Laboratory
ORNL	Oak Ridge National Laboratory

Associated Publications

Publication Id
No data to show.

Feedstocks

Feedstock Type
Corn Stover

Products

Product Type
No data to show.

Technology Pathways

Technology Pathway
Low Temperature Conversion & Upgrading of Dry Feedstock

Process Areas

Process Area
Feedstock Supply & Logistics

Relevant Unit Operations

Unit Operation
Baling
Collection
Field Side Storage



2 – Progress – Improved design and dynamic content to introduce stakeholders to FCIC Subtask Teams

T.03.05.P1 Bulk Flow Characterization

Subtask Overview

Subtask Description

Description

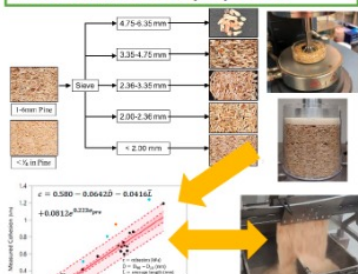
The objectives of this subtask are to measure physical and mechanical properties of biomass to accurately represent their stress-strain and flow behavior in addition to quantify with varied MAs to supply FEM/DEM models qualitative and quantitative flow characteristics in shear testers as well as hopper and auger unit operations. Another outcome from this work will be to develop and disseminate a methods roadmap, in collaboration with all Subtask 3.5 stakeholders, for characterizing critical flow parameters of novel feedstocks. The major subtask outcomes will be to identify MAs impacts on bulk shear and flow performance (CQA) and provide model validation and calibration data sets for subtasks 3.1, 3.2, and 3.3 in coordination with the other experimental tasks 3.4 and 3.6. This will lead to the ability to design biomass conveyance systems for a wide range of operational conditions and materials in coordination with the modeling outcomes.

Knowledge and Tools (scroll down)

Multiscale bulk flow characterization



Developed relationships between material attributes and resulting shear and bulk flow properties.



Current Knowledge Gap

- Current state-of-the-art particle mechanics and granular flow models were developed in soil mechanics with test methods appropriate for incompressible, regular solids.
- These test methods do not directly extract equivalent properties for biomass because of the complex interactions of biomass anisotropic compressibility, bulk creep, surface properties and morphology, and heterogeneity/variability.
- Current quasi-static test methods and properties do not directly predict or indicate flow performance in pilot equipment such as has been developed for powders and solids.

Achievement

- Develop multiscale characterization methods and pair with flow validation data to correlate material attributes with bulk flow performance, and lab-scale flow inception and critical state shear properties.

Relevance

- Understanding how characterization methods and material properties

Management Details - Publications - Topic Areas

Study Short Name	Label	Start Date	End Date	Investigator	POC1	POC2
<T.03.05.P1>	T.03.05.P1 Bulk Flow Characterization	2018-10-01 00:00		Jordan Klinger	Jordan Klinger	Troy Semelsberger

Participating Organizations	Name
INL	Idaho National Laboratory
NREL	National Renewable Energy Laboratory
PNNL	Pacific Northwest National Laboratory

Publications

Impacts of Biological Heating and Degradation during Bale Storage on the Surface Properties of Corn Stover
A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine
A Review of Computational Models for the Flow of Milled Biomass Part II: Continuum Mechanics Models
A Review of Computational Models for the Flow of Milled Biomass

Feedstock Types

Corn Stover
Loblolly Pine

Product Types

Diesel Blendstock
Gasoline Blendstock

Technology Pathway

Direct Liquefaction & Upgrading of Dry Feedstock
Low Temperature Conversion & Upgrading of Dry Feedstock

QbD Process Parameter

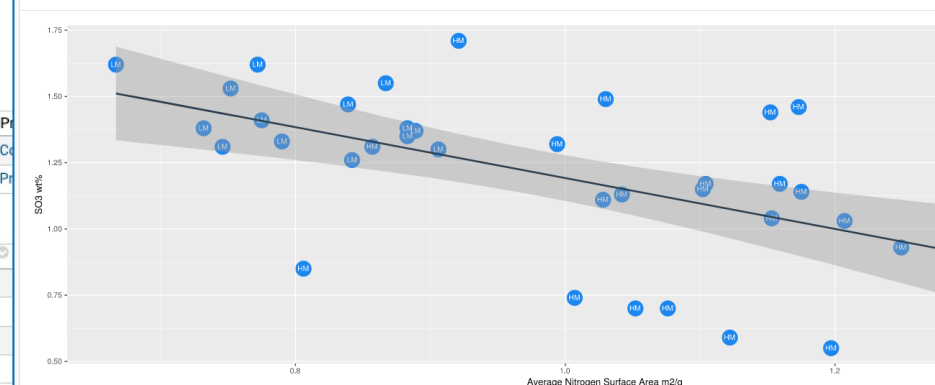
Feed Rate
Material Of Construction
Wall Construction
Wall Geometry

QbD Process Stream Property

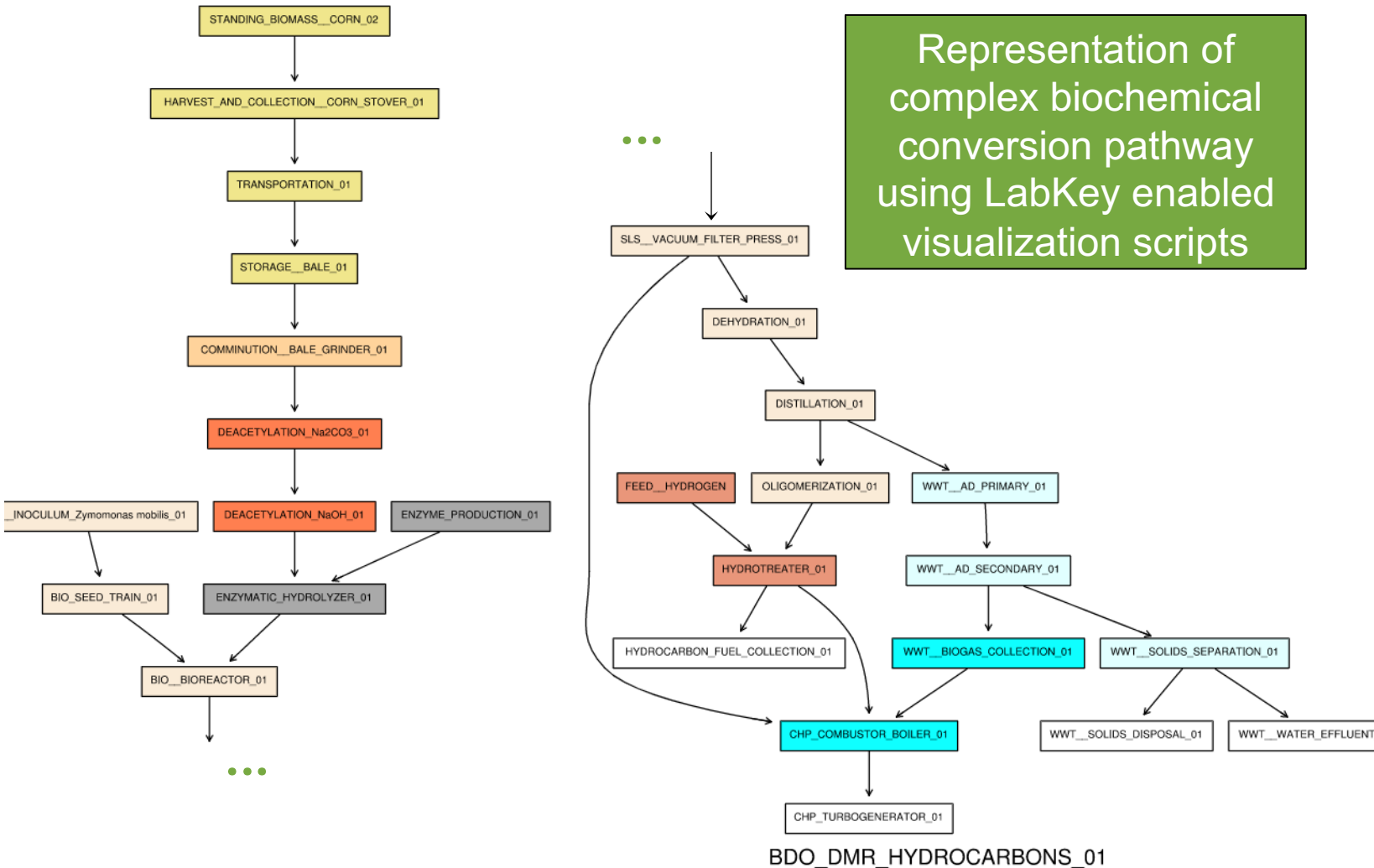
Bulk Density
Cohesive Strength
Compressibility
Mass Flow

T.03.05.P1 Bulk Flow Characterization

N2 Surface Area vs. SO3 Content



2 – Progress – Rapid composition and display of technology pathways from QbD data tables



Description

A new tool on the [FCIC Data Hub](#) enables users to **rapidly compose and visualize technology pathways** from a standardized set of unit operations linked to FCIC data.

Value of new tool

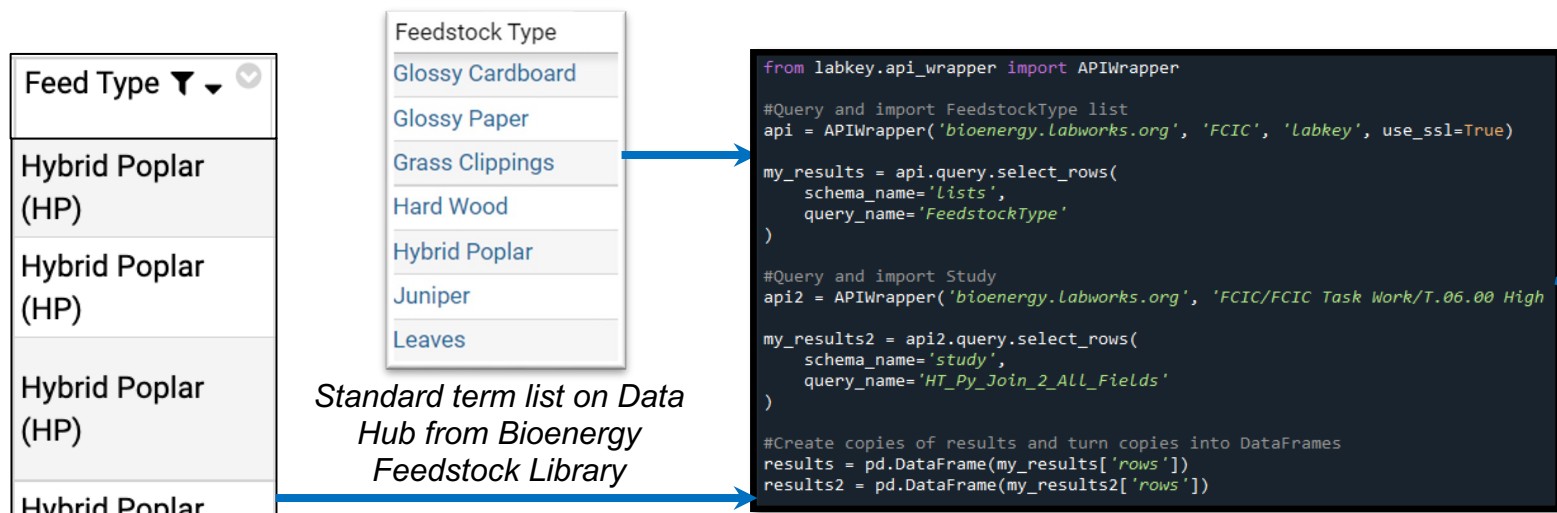
This new tool organizes and presents biorefinery designs, unit operations, and performance data within a **standardized Quality by Design (QbD) framework**. Industry stakeholders save time by viewing and downloading FCIC data that have been made **Findable, Accessible Interoperable, and Reusable (FAIR)**.

Industry Impact

The technology pathway composition and rendering tool has been [deployed on the Data Hub](#). Work is underway to display hyperlinked QbD data on the pathway diagrams.



2 – Progress – Automated harmonization of data terms using the Record Linkage Toolkit



The **Python Record Linkage Toolkit*** is a library to link records in or between data sources. The toolkit provides most of the tools needed for record linkage and deduplication. The package contains indexing methods, functions to compare records and classifiers. With it you can:

- Clean and standardize data.
- Make pairs of records using smart indexing methods such as **blocking** and **sorted neighborhood indexing**
- Compare records using many comparison and similarity measures for different types of variables such as strings, numbers and dates.
- Perform classifications using both supervised and unsupervised algorithms.

Nonstandard terms in datasets coming from multiple experimental teams

HP Feed Type	FT Feed Type
Hybrid Poplar	Hybrid Poplar (HP)
Hybrid Poplar	Hybrid Poplar (HP)
Hybrid Poplar	Hybrid Poplar (HP)
Hybrid Poplar	Hybrid Poplar
Hybrid Poplar	Hybrid Poplar
Hybrid Poplar	HP F5H

Nonstandard terms are automatically mapped to standard terms

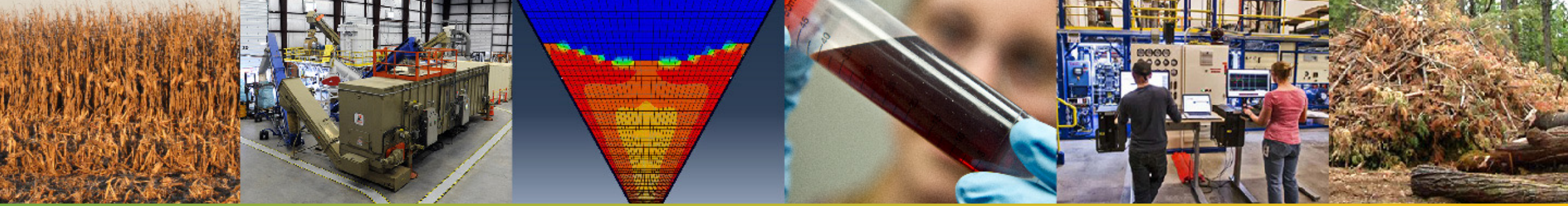
Python script (Devin Power, PNNL)

Index	Index	Feed Type
6	8	1
6	58	1
6	59	1
6	60	1
6	61	1

Indexing and Classification

*<https://recordlinkage.readthedocs.io/en/latest/about.html>
© Copyright 2016-2022, Jonathan de Bruin Revision bd5cd08a
Free, open-source code under GPLv3 and BSD-3-Clause licenses





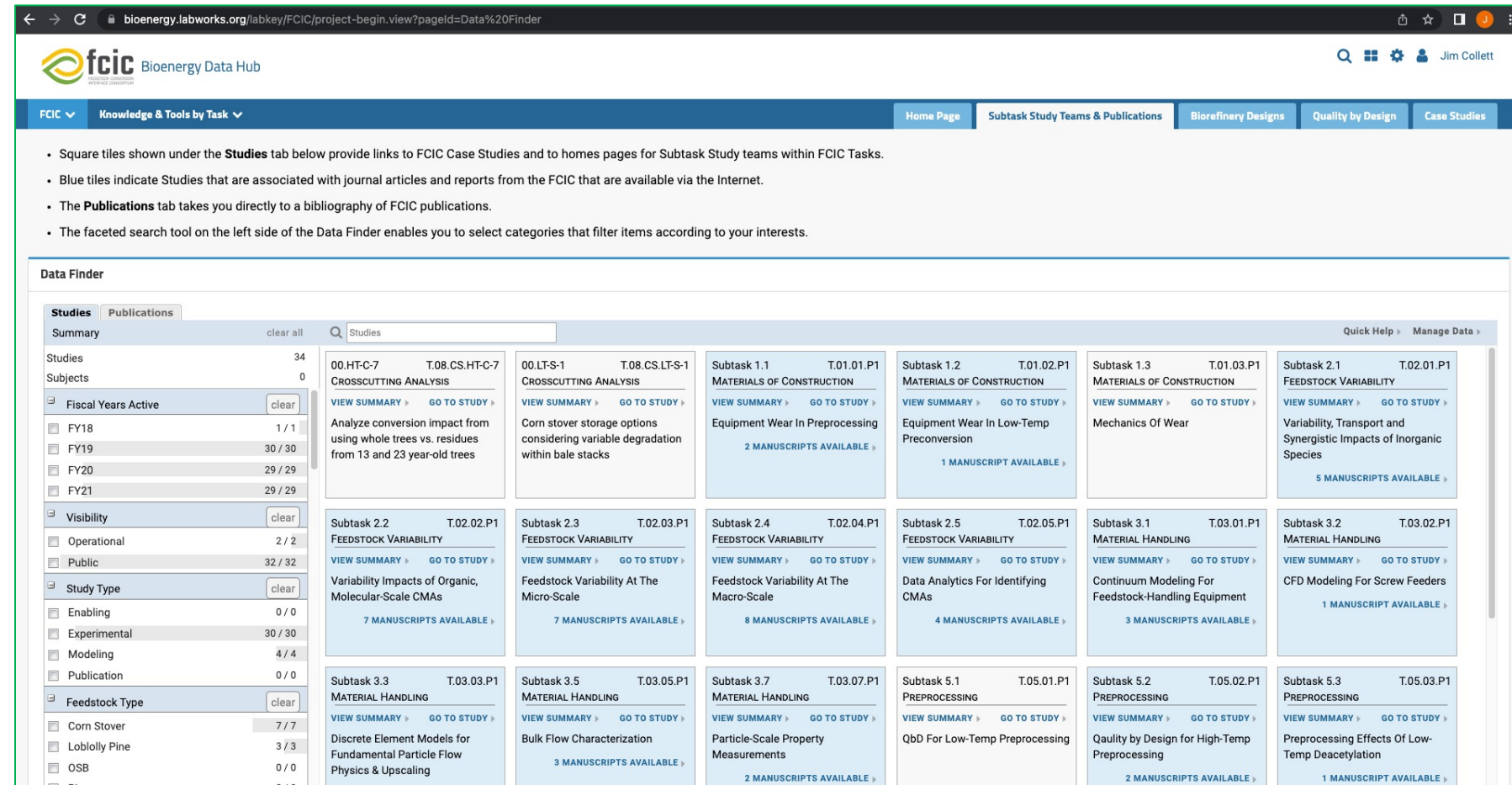
3 – Impact

- Industrial stakeholders will have access to:
 - A modern, commercial-quality collaborative platform to integrate, standardize, and archive datasets for advanced analytics and TEA/LCA.
 -
 - A web portal with advanced search tools for sharing FCIC datasets with industrial stakeholders.
 - A “one-stop-shop for accessing FCIC Case Studies, journal articles, datasets, and info briefs (i.e., K&T slides).
- The Data Hub’s QbD database and searchable Subtasks and publications will provide well-documented data and evidence for:
 - Material properties for biorefinery feedstocks, intermediates, and products.
 - Process parameters for commercial unit operations to facilitate biorefinery scale-up.
 - Data that can support market specifications for feedstocks, intermediates, and products throughout the value chain.



3 – Impact – Dissemination

- We will promote the FCIC Data Hub as the "go-to" platform for datasets on feedstock variability and biorefinery unit operations via webinars, publications, and conference presentations.
- High quality, curated datasets on the Data Hub will be convincing "calling cards" for industrial partnerships that lead to commercialization and deployment of BETO-funded research.



The screenshot displays the FCIC Bioenergy Data Hub interface. At the top, there's a navigation bar with the FCIC logo and the text "Bioenergy Data Hub". Below this is a "Data Finder" section. On the left, there's a sidebar with filters for "Studies" and "Publications". The main area shows a grid of study tiles, each representing a different subtask or task. Each tile includes a title, a brief description, and a link to "VIEW SUMMARY" or "GO TO STUDY". The tiles are organized into rows and columns, with some tiles indicating the number of manuscripts available.

Key features visible in the interface include:

- Search Bar:** A search bar at the top right of the main content area.
- Filters:** A sidebar on the left with filters for "Studies" and "Publications".
- Study Tiles:** A grid of study tiles, each representing a different subtask or task. Each tile includes a title, a brief description, and a link to "VIEW SUMMARY" or "GO TO STUDY".
- Manuscript Availability:** Some tiles indicate the number of manuscripts available, such as "2 MANUSCRIPTS AVAILABLE" or "1 MANUSCRIPT AVAILABLE".

Data Finder interface on the home page of the FCIC Data Hub at <https://bioenergy.labworks.org/labkey/FCIC/project-begin.view?pagelD=Data%20Finder>



3 – Impact – AI innovations such as ChatGPT create new opportunities and risks for FCIC data access

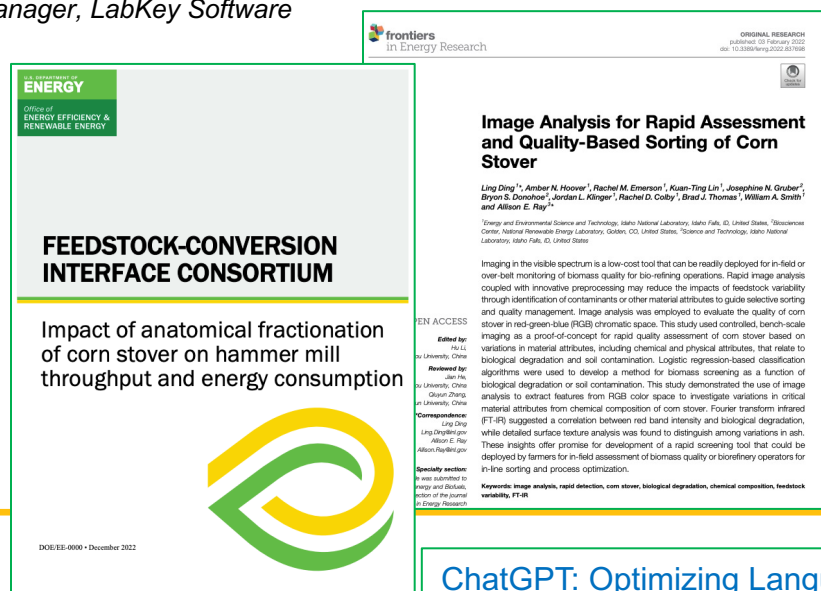


A ChatGPT response to the question “**What are the critical quality attributes [CQAs] when converting corn stover into biofuel?**”*

suggested that their algorithm drew heavily from FCIC publications that are freely available on the Internet.

We are examining the benefits and risks of such online AI tools to enhance the accessibility and utility of FCIC data and information while maintaining stakeholder confidence in our work.

*Performed in collaboration with Steve Hanson, Technical Account Manager, LabKey Software



ChatGPT response to specific question on CQAs of corn stover for biofuels

chat.openai.com/chat/e0653439-f676-4f6f-8359-158815028973

What are the critical quality attributes when converting corn stover into biofuel?



The critical quality attributes (CQAs) of corn stover for biofuel production depend on the specific conversion process and end-product goals. However, some general CQAs that are often considered for corn stover feedstocks include:

1. Moisture content: High moisture content can reduce the efficiency of conversion processes and increase transportation costs.
2. Ash content: High levels of ash can lead to equipment corrosion and reduce the energy content of the feedstock.
3. Cellulose, hemicellulose, and lignin content: These are the primary components of corn stover and affect the efficiency and yield of conversion processes. Generally, higher cellulose and hemicellulose content is desirable, while lignin can be more difficult to break down.
4. Sugar content: The amount of fermentable sugars in the corn stover affects the potential yield of biofuels such as ethanol.
5. Particle size and uniformity: Small and uniform particle size can improve the efficiency of conversion processes and reduce processing costs.
6. Purity and contaminants: Contaminants such as rocks, dirt, and metals can damage processing equipment and reduce the efficiency of conversion processes.
7. Sustainability: The environmental impact of corn stover production and conversion should also be considered, including water use, and greenhouse gas emissions.

In this case, ChatGPT provided a surprisingly useful—but uncredited—summation of CQAs.

3 – Impact – The FCIC is democratizing access to harmonized bioenergy data to accelerate profitable biorefinery deployment

FY21 Peer Review Feedback:

“The project is very ambitious in the amount of data and information it is encompassing. Standardizing QbD nomenclature as well as linking to other programs such as the Bioenergy Feedstock Library will be key to institutionalizing the concept across FCIC.”

“...the challenge will be to get industry and even other technology areas of BETO to adopt the standardized nomenclature and start using the data sets and reports.”



Center for
Open
Science's
strategy for
culture
change



<https://www.cos.io/blog/strategy-for-culture-change>

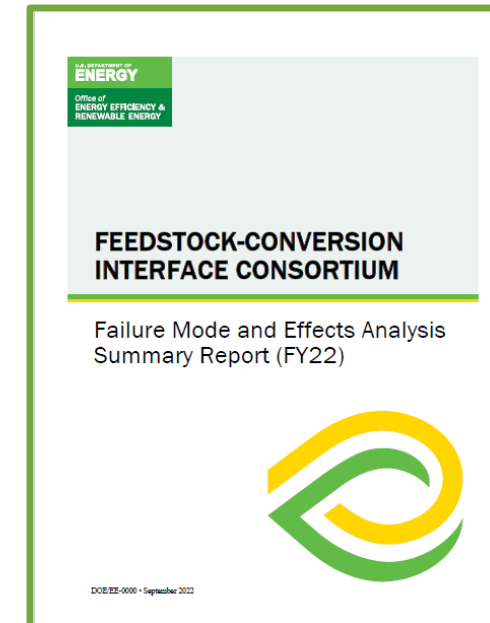
3 – Impact – Supporting FCIC Publications and Report

The Data Hub's LabKey infrastructure was used to support Failure Mode Effects Analysis that was performed under Task 9, resulting in the following publication:

- Emerson, Rachel M, Burli, Pralhad Hanumant, Vega Montoto, Lorenzo J, and Bhattacharjee, Tiasha. *FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM: Failure Mode and Effects Analysis Summary Report (FY22)*. United States: N. p., 2022. Web. doi:[10.2172/1894327](https://doi.org/10.2172/1894327).

This database contains all of the FMEA results collected to date. To see details regarding the FMEA SME interview result the detailed FMEA interview summaries.

	Unit Operation	Equipment Type	Material Stream	Tech Pathway	Process Flow Diagram RT	Failure	TRL	Severity	Occurrence	Detection	RPN	CQA Material	Units	CQA Pro
<input type="checkbox"/>	FRACTIONATION_AIR_CLASSIFIER_03	Air Classifier	Pine Residue	FMEA_HT-P-1		Partially blocked screen_01	A	10	3	10	300	ASH_CONTENT_01	%	
<input type="checkbox"/>	FRACTIONATION_AIR_CLASSIFIER_03	Air Classifier	Pine Residue	FMEA_HT-P-1		Partially blocked screen_01	A	10	3	10	300	PARTICLE_SIZE_01	mm	



Technical Approach

- Deploy the FCIC Bioenergy Data Hub using the open source [LabKey web application platform](#) to make FCIC data and information **F**indable, **A**ccessible, **I**nteroperable, and **R**eusable (FAIR) in accordance with the DOE Office of Science and Technology Information's [Research Data Management Policy](#).

Impact

- The 3-year outcome of this Task will be to establish an online community of industry of stakeholders, National Lab researchers, and BETO staff sharing data, knowledge, and tools via the FCIC Data Hub. All FCIC Integrated Analysis Task Case Studies, publications, QbD properties and supporting information data produced by the FCIC will be available to industry stakeholders via the Data Hub, with a target of having 100+ active users from commercial entities.

Achievements

- The FCIC Data Hub has been opened to non-DOE users on a limited basis for beta testing. It contains 8 Case Studies with QbD-harmonized datasets ready for downloading; one-stop bibliographic access to more than 80 FCIC journal articles and technical reports; and 135 Knowledge & Tool slides. Full opening planned for FY23.
- The FCIC Data Stakeholder Advisory Panel was convened for guidance on Data Hub design, function, and content.
- Improved web design and dynamic content tools created to introduce stakeholders to FCIC Subtask Teams and their work.
- New Tools for rapid composition and dynamic display of biorefinery Technology Pathways from unit operation and QbD data tables.
- Automated Harmonization to Standard Data Terms using the Record Linkage Toolkit
- Analysis of how 3rd-party online AI innovations such as ChatGPT will influence interpretation of FCIC knowledge products.



Quad Chart Overview

Timeline

- *October 1, 2021*
- *September 30, 2024*

	FY22 Costed	Total Award
DOE Funding	\$550K	\$1650K
Project Cost Share *	NA	NA

TRL at Project Start: 2
TRL at Project End: 8

Project Goal

Provide a modern, collaborative computational environment for hypothesis development, experimental and modeling workflow management, integration of datasets and metadata, and deliverables sharing between FCIC subtasks within a uniform Quality by Design framework, as well as a portal for public access to FCIC results, data, and software.

End of Project Milestone

Realization of an online community of industry stakeholders, National Lab researchers, academic partners, and BETO staff who share data, knowledge, via the FCIC Data Hub with a target of having 100+ active users from commercial entities.

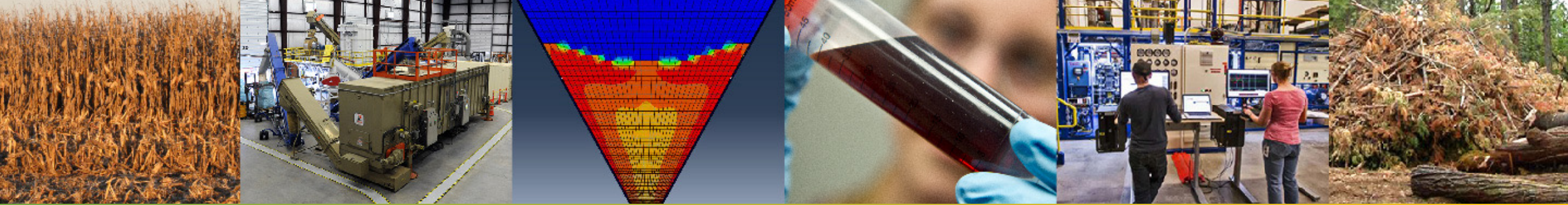
Funding Mechanism

2021 Lab Call – FCIC Merit Review

Project Partners*



*Only fill out if applicable.



Additional Slides

2 – Progress –Task 4 Milestones

FY22 Q1 (PNNL) Data Hub Ingestion and Harmonization of Task 8 Data Sheets; form Data Stakeholder Advisory Team	Harmonization and database ingestion of parameters, data types, and units of measure for Case Study Data Information Sheets generated by Task 8-led planning for FY22 TEA with Experimental Task Teams. Data Stakeholder Advisory Team formed for feedback and guidance on industry relevance of Data Hub resources, formats, and standards.	12/31/21 Complete
FY22 Q2 (INL): Case Studies Data Hub Integration and Publication	Integrate 2 Preprocessing focused Case Studies (batch 1) into Data Hub to support Task 8 presentation of live data tables, visualizations, and narratives to Data Stakeholder Advisory Team.	3/31/22 Complete
FY22 Q3 (NREL): Case Studies Data Hub Integration and Publication	Integrate 2 Conversion focused Case Studies (batch 2) into Data Hub to support Task 8 presentation of live data tables, visualizations, and narratives to Data Stakeholder Advisory Team.	6/30/22 Complete
FY22 Q4 (PNNL): Data Stakeholder Workshop	Inaugural annual Data Stakeholder workshop and training conducted using the Data Hub live for Case Study reviews, platform evaluation and feedback, and training. <i>(delayed while National Lab information release processes are being harmonized)</i>	9/30/22 Delayed
FY23 Q1 (INL) Integration of FY22 material Needs with core FCIC datasets and metadata	Integration of FY22 Material Needs with core FCIC datasets and metadata for preprocessed feedstocks within the Data Hub to link data to R&D tasks and Case Studies and facilitate access for online analysis and downloading by industrial stakeholders.	12/31/22 Complete
FY23 Q2 (PNNL) Data Stakeholder Focus Groups	Provide Data Hub user accounts to at least 20 non-DOE stakeholders and conduct 3 focus group sessions to collect in-person feedback on the web portal's performance and utility.	3/31/23
FY23 Q3 (NREL/INL) Task 8 Case Study Support	LabKey "Study" home folders created for 4 new Task 8 Case Studies and two high-profile FCIC publications with data, metadata, and results integrated within the FCIC QbD database.	6/30/23
FY24 Q4 (PNNL) FCIC Data Stakeholder Workshop Planning	Agenda, guest speakers, and discussion sessions outlined for FCIC Data Stakeholder Workshop; Demonstrate QbD technology pathway critical properties rendering tool.	9/30/23
FY24 Q4 (PNNL) 3-year Final Deliverable	An online community of industry of stakeholders, National Lab researchers, academic partners, and BETO staff sharing data, knowledge, and tools is established on the FCIC Data Hub with a target of having 100+ active users from commercial entities.	9/30/24



- *Comment, Reviewer 1:* A huge undertaking within BETO that is clearly advancing towards its goal of a comprehensive data hub. From other presentations it appears that some datasets are going to be added onto this with different UI / layouts. If true, this would harm the overall effort of a consistent platform. The data needs to be accessed, entered, and viewed in a consistent manner to give people confidence that the data is accurate as well as to provide a consistency in quality required for such an effort....Recommend that only a small group of people be allowed to make data entries instead of anyone. Data can and will likely be entered sloppily by users in a rush to get the menial task over with. However, if a group of people had sole control, they could ensure that the data was equivalent, definitions were consistent, and experiments were taking the correct measurements. The project is not only for the final depository of data but could be used as a project planning tool as well. It has the potential to help guide projects towards the correct items to measure in their labs, and in their processes....This tool should be used as a specification for data collection for government projects. The same data, collected in the same ways, done on each project is the most important way of making this dataset valuable. A publicly available tool which can provide data on a particular feedstock at a particular point in a system that has been vetted by national lab scientists is an exciting advancement.
- *Response:* We agree that maximizing the value of the Bioenergy Data Hub will require researchers working across the nine National Labs of the FCIC to agree upon and adhere to common standards for material and process data and metadata to ensure that their uploaded datasets will be findable, accessible, interoperable, and reusable by our industry stakeholders. A key, measurable objective for our Task will be to harmonize datasets from FCIC technical reports and journal articles, and then upload them to the Data Hub to enable integrated views of FCIC data within a single interface with standardized metadata and units of measure. Workflows for achieving such data integration will necessarily involve only a small, select group of data managers from each of the FCIC National Labs to ensure data quality.



- *Comment:* The project is very ambitious in the amount of data and information it is encompassing. Standardizing QbD nomenclature as well as linking to other programs such as the Bioenergy Feedstock Library will be key to institutionalizing the concept across FCIC. Although this effort is great for FCIC internal collaboration, the challenge will be to get industry and even other technology areas of BETO to adopt the standardized nomenclature and start using the data sets and reports. The beta testing using the IAB and getting input from the DFO partners is a good start. Ease of use will be key to the adoption of this technology. The data set on High-Temperature Conversion does not have any DFO or industry partner using the pyrolysis technology for the production of biofuels. This will limit the applicability of the current data sets in this space. More extensive input from industry as well as Beta-testing by industry users will be key to determining the value to the biorefinery community.
- *Response:* Our uniform applications of Quality by Design (QbD) nomenclature within the Process Stream Critical Properties, Unit Operation Critical Process Parameters, and Technology Pathway Configuration data tables on the Data Hub are indeed standardizing the way we think and talk about biorefinery materials and processes within the FCIC. Further integration of the FCIC's QbD framework for biorefineries with the database schema of the BFL can form the basis of a new "Bioeconomy Feedstock Conversion Ontology" that provides a shareable and reusable framework of formally specified objects, classes, attributes, and relations to support biorefinery development and the creation of markets for renewable feedstocks, intermediates, and products.

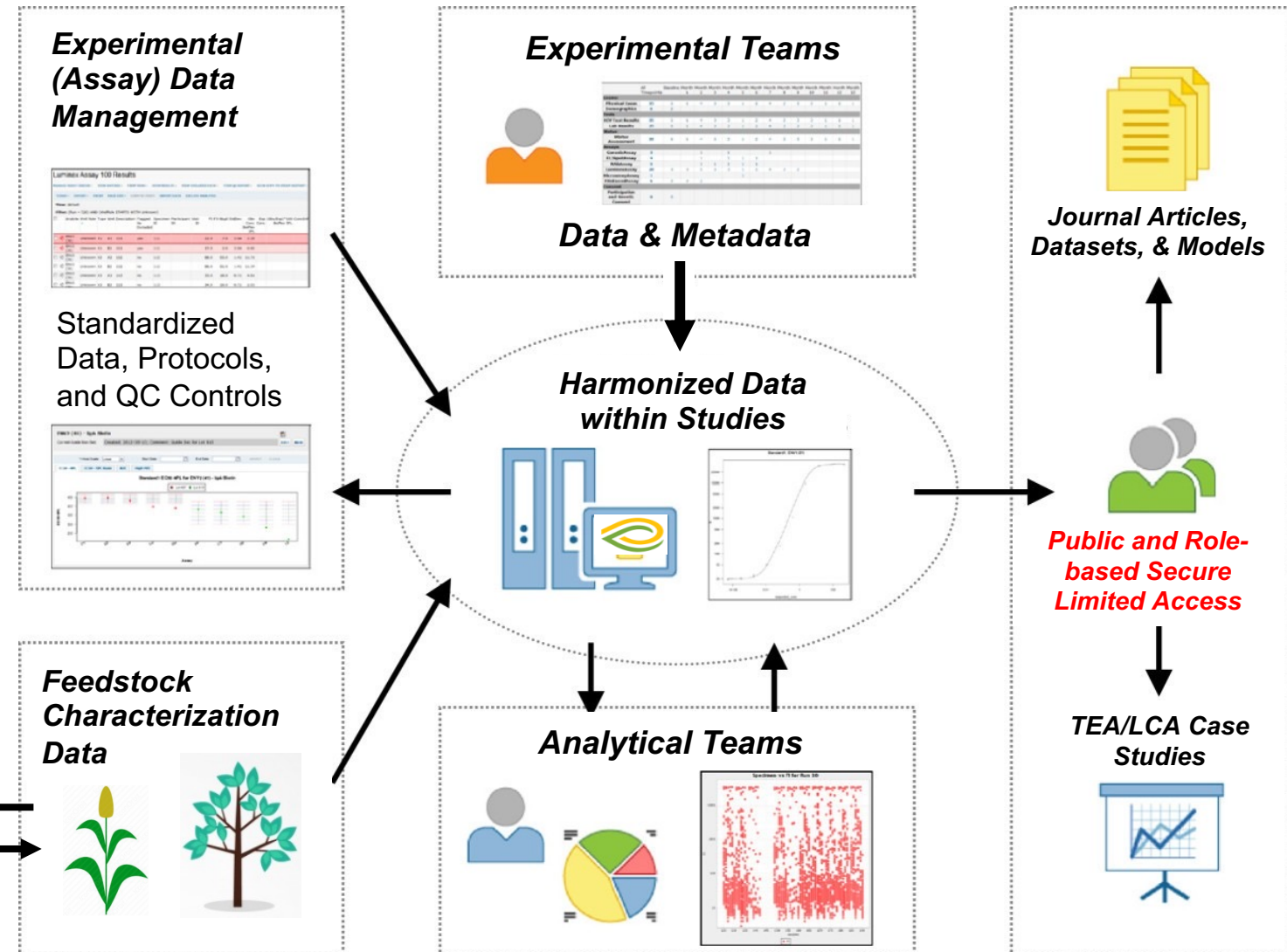


1 – Approach

LabKey Data Server Infrastructure:

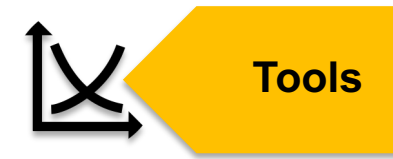
- We are leveraging LabKey's built-in workflows to **integrate bench-to-PDU scale feedstock and experimental data** within "Study" data structures.
- The FCIC's 34 **Subtasks** have their own **Study folders** wherein datasets, statistical views of the data, figures, and text may be collaboratively compiled into publications that provide standardized, downloadable datasets.
- Access is provided to the public following all **National Lab and DOE information release policies**; secure access to selected content may be provided to specific industrial, academic, and NL partners using LabKey's extensive **role-based permissions*** system.

*LabKey user roles include FCIC Data Hub Admins, Editors, Analysts (can create and enable script code) and Readers. Roles may be assigned on a per-folder basis for granular access permission assignment.



Adapted from BMC Bioinformatics volume 14, Article number: 145 (2013)

4 – Progress: Bioenergy Feedstock Library integration via Python API



Creation of LabKey Datasets directly from Bioenergy Feedstock Library (BFL) exports

BFL Export

Sample ID	Date	BFL Sample Identifier	BFL Metadata Project	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation
17f5b32c-4PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
10f9e894-7699-4224-9162-70048f2a5661	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
35874113-PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
764051f5-PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
2b2088a5-PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
4b6c7249-PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
45e7799b-PDU User fGeneral	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										

LabKey Data Set

Dataset: Lot10_BFLtoLabKey.xlsx

Contains up to one row of Lot10_BFLtoLabKey.xlsx data for each SampleID/BFL_GUID combination.

Sample ID	Date	BFL Sample Identifier	BFL Metadata Project	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation	BFL Metadata Equipment	BFL Metadata Operation
10f9e894-7699-4224-9162-70048f2a5661	2020-03-12	10f9e894-7699-4224-9162-70048f2a5661	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										
2470c701562a24a6435908c596c7a	2020-03-12	2470c701562a24a6435908c596c7a	PDU User Facility	Grinding	Grinder	Vermeer B Pulled Grab sample w 18f1e035-13.8	Freddie DuArrived at 1 gallon baStory	2014	Corn St										

Description

LabKey's Python API was used to develop an automated process for creating Study datasets for batches of sample provenance and analytical data exported from the Bioenergy Feedstock Library (BFL).

Value of new tool

The tool reduces the need to manually create redundant data structures between the two systems and represents an additional method to establish interoperability between the BFL and LabKey.

Potential Customers & Outreach Plan

INL researchers can more easily import samples and data directly into LabKey that are being tracked for the FCIC in the BFL database system.



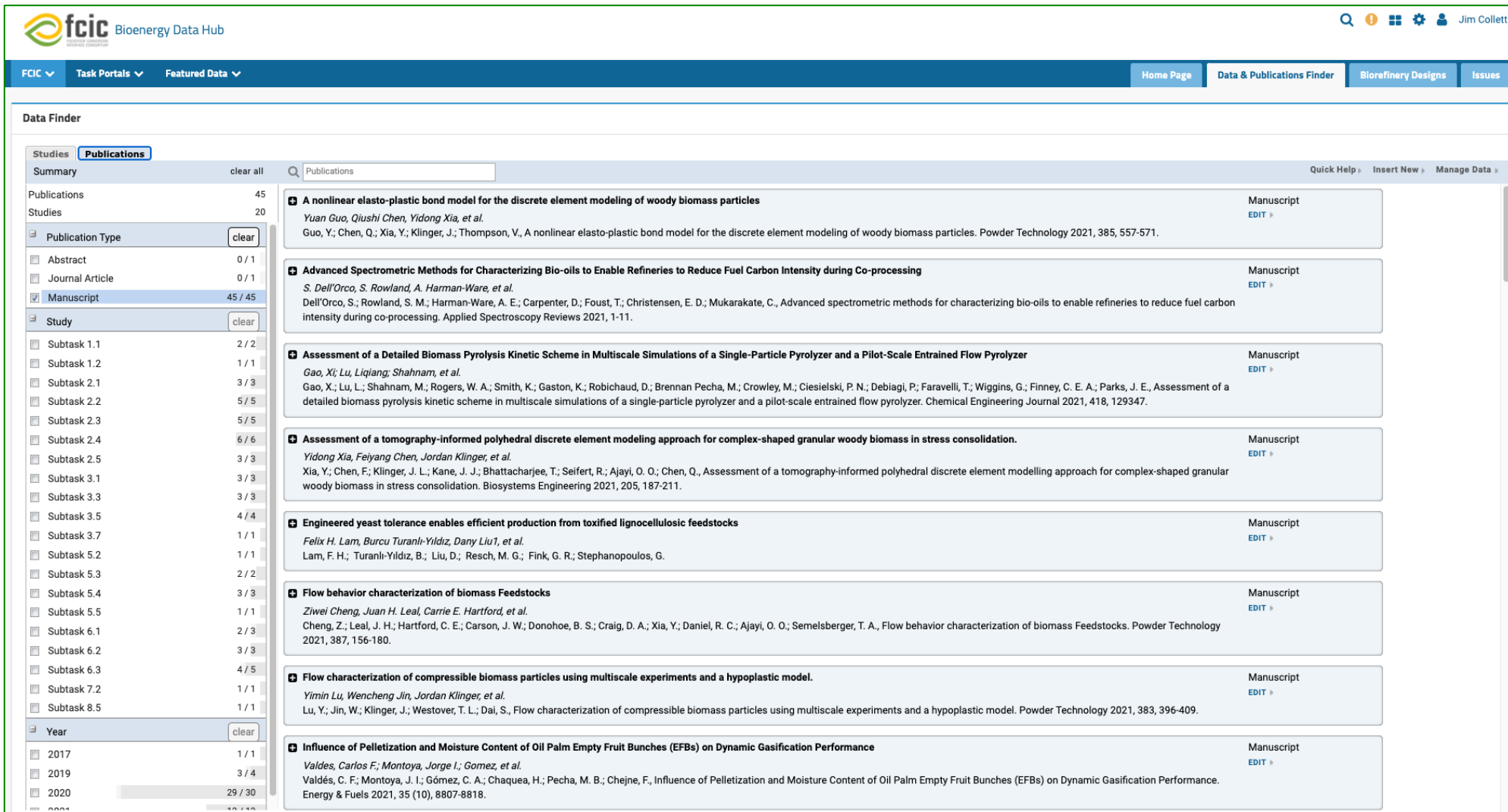
4 – Progress: Finding Knowledge and Tools on the FCIC Data Hub



- The Data Hub Web Portal is now online and equipped with a “Data Finder” dashboard for accessing “Study” folders for each FCIC Subtask. FCIC publications may be accessed via the “Publications” tab.
- Data accruing on the Data Hub are easily **Findable** and **Accessible** (per FAIR data guidelines) via a faceted search tool that allows users to click on metadata tags to rapidly down-select to Subtasks covering specific R&D focus areas.

Subtask metadata tags now include a range of 260 descriptors for analytical methods, feedstock types, product types, technology pathways, process areas, unit operations, process parameters, process stream properties, fiscal years active, and participating organizations.

Data Finder Publications Tab



The screenshot shows the FCIC Bioenergy Data Hub interface. The top navigation bar includes the FCIC logo, "Bioenergy Data Hub", and user information "Jim Collett". Below this is a secondary navigation bar with tabs: "FCIC", "Task Portals", "Featured Data", "Home Page", "Data & Publications Finder" (selected), "Biorefinery Designs", and "Issues".

The main content area is titled "Data Finder" and contains a sidebar on the left and a main list of publications on the right.

Left Sidebar:

- Studies** (selected): Publications (45), Studies (20)
- Publication Type** (clear):
 - ☐ Abstract (0 / 1)
 - ☐ Journal Article (0 / 1)
 - ☒ Manuscript (45 / 45)
- Study** (clear):
 - Subtask 1.1 (2 / 2)
 - Subtask 1.2 (1 / 1)
 - Subtask 2.1 (3 / 3)
 - Subtask 2.2 (5 / 5)
 - Subtask 2.3 (5 / 5)
 - Subtask 2.4 (6 / 6)
 - Subtask 2.5 (3 / 3)
 - Subtask 3.1 (3 / 3)
 - Subtask 3.3 (3 / 3)
 - Subtask 3.5 (4 / 4)
 - Subtask 3.7 (1 / 1)
 - Subtask 5.2 (1 / 1)
 - Subtask 5.3 (2 / 2)
 - Subtask 5.4 (3 / 3)
 - Subtask 5.5 (1 / 1)
 - Subtask 6.1 (2 / 3)
 - Subtask 6.2 (3 / 3)
 - Subtask 6.3 (4 / 5)
 - Subtask 7.2 (1 / 1)
 - Subtask 8.5 (1 / 1)
- Year** (clear):
 - 2017 (1 / 1)
 - 2019 (3 / 4)
 - 2020 (29 / 30)

Main List of Publications:

- 1 A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles**
Yuan Guo, Qilishi Chen, Yidong Xia, et al.
Guo, Y.; Chen, Q.; Xia, Y.; Klinger, J.; Thompson, V., A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles. Powder Technology 2021, 385, 557-571. Manuscript EDIT
- 2 Advanced Spectrometric Methods for Characterizing Bio-oils to Enable Refineries to Reduce Fuel Carbon Intensity during Co-processing**
S. Dell'Orco, S. Rowland, A. Harman-Ware, et al.
Dell'Orco, S.; Rowland, S. M.; Harman-Ware, A. E.; Carpenter, D.; Foust, T.; Christensen, E. D.; Mukarakate, C., Advanced spectrometric methods for characterizing bio-oils to enable refineries to reduce fuel carbon intensity during co-processing. Applied Spectroscopy Reviews 2021, 1-11. Manuscript EDIT
- 3 Assessment of a Detailed Biomass Pyrolysis Kinetic Scheme in Multiscale Simulations of a Single-Particle Pyrolyzer and a Pilot-Scale Entrained Flow Pyrolyzer**
Gao, Xi; Lu, Liqiang; Shahnam, et al.
Gao, X.; Lu, L.; Shahnam, M.; Rogers, W. A.; Smith, K.; Gaston, K.; Robichaud, D.; Brennan Pecha, M.; Crowley, M.; Ciesielski, P. N.; Debiagi, P.; Faravelli, T.; Wiggins, G.; Finney, C. E. A.; Parks, J. E., Assessment of a detailed biomass pyrolysis kinetic scheme in multiscale simulations of a single-particle pyrolyzer and a pilot-scale entrained flow pyrolyzer. Chemical Engineering Journal 2021, 418, 129347. Manuscript EDIT
- 4 Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation.**
Yidong Xia, Feiyang Chen, Jordan Klinger, et al.
Xia, Y.; Chen, F.; Klinger, J. L.; Kane, J. J.; Bhattacharjee, T.; Seifert, R.; Ajayi, O. O.; Chen, Q., Assessment of a tomography-informed polyhedral discrete element modelling approach for complex-shaped granular woody biomass in stress consolidation. Biosystems Engineering 2021, 205, 187-211. Manuscript EDIT
- 5 Engineered yeast tolerance enables efficient production from toxified lignocellulosic feedstocks**
Felix H. Lam, Burcu Turanli-Yildiz, Dany Liu1, et al.
Lam, F. H.; Turanli-Yildiz, B.; Liu, D.; Resch, M. G.; Fink, G. R.; Stephanopoulos, G. Manuscript EDIT
- 6 Flow behavior characterization of biomass Feedstocks**
Ziwei Cheng, Juan H. Leal, Carrie E. Hartford, et al.
Cheng, Z.; Leal, J. H.; Hartford, C. E.; Carson, J. W.; Donohoe, B. S.; Craig, D. A.; Xia, Y.; Daniel, R. C.; Ajayi, O. O.; Semelsberger, T. A., Flow behavior characterization of biomass Feedstocks. Powder Technology 2021, 387, 156-180. Manuscript EDIT
- 7 Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model.**
Yimin Lu, Wencheng Jin, Jordan Klinger, et al.
Lu, Y.; Jin, W.; Klinger, J.; Westover, T. L.; Dai, S., Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model. Powder Technology 2021, 383, 396-409. Manuscript EDIT
- 8 Influence of Pelletization and Moisture Content of Oil Palm Empty Fruit Bunches (EFBs) on Dynamic Gasification Performance**
Valdes, Carlos F.; Montoya, Jorge I.; Gomez, et al.
Valdés, C. F.; Montoya, J. I.; Gómez, C. A.; Chacuea, H.; Pecha, M. B.; Chejne, F., Influence of Pelletization and Moisture Content of Oil Palm Empty Fruit Bunches (EFBs) on Dynamic Gasification Performance. Energy & Fuels 2021, 35 (10), 8807-8818. Manuscript EDIT

- Detailed information about FCIC publications may be found under the Publications tab of the Data Finder.



4 – Progress: LabKey Subtask Studies



Technical Approach:

- Each of the FCIC's 35 Subtasks has its own "Study" home page on the Data Hub
- Studies have links for datasets, analyzed data views, results narratives, provenance, publications, and metadata associated with the Subtask.
- Subtask Studies provide supporting data and information for the 66 "Knowledge" and "Tool" products developed thus far by the FCIC.

Overview: /FCIC/FCIC Task W: x +

bioenergy.labworks.org/labkey/FCIC/FCIC%20Task%20Work/T.03.00%20Materials%20Handling/T.03.05.P1%20Bulk%20Flow%20Characterization/project-begin.view?

fcic Bioenergy Data Hub

FCIC Task Portals Studies

T.03.05.P1 Bulk Flow Characterization

Subtask Description

Subtask Description

Description

The objectives of this subtask are to measure physical and mechanical properties of biomass to accurately represent their stress-strain and flow behavior in addition to quantify with varied MAs to supply FEM/DEM models qualitative and quantitative flow characteristics in shear testers as well as hopper and auger unit operations. Another outcome from this work will be to develop and disseminate a methods roadmap, in collaboration with all Subtask 3.5 stakeholders, for characterizing critical flow parameters of novel feedstocks. The major subtask outcomes will be to identify MAs impacts on bulk shear and flow performance (COA) and provide model validation and calibration data sets for subtasks 3.1, 3.2, and 3.3 in coordination with the other experimental tasks 3.4 and 3.6. This will lead to the ability to design biomass conveyance systems for a wide range of operational conditions and materials in coordination with the modeling outcomes.

Subtask Topics, Publications, and Provenance

Management Details

Study Short Name	Label	Start Date	End Date	Investigator	POC1	POC2
T.03.05.P1	T.03.05.P1 Bulk Flow Characterization	2018-10-01 00:00		Jordan Klingler	Troy Semelsberger	

Participating Organizations

Participating Organizations	Name
INL	Idaho National Laboratory
NREL	National Renewable Energy Laboratory
PNNL	Pacific Northwest National Laboratory

Subtask Publications

Publications

- Impacts of Biological Heating and Degradation during Bale Storage on the Surface Properties of Corn Stover
- A density-dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine
- A Review of Computational Models for the Flow of Milled Biomass Part II: Continuum-Mechanics Models
- A Review of Computational Models for the Flow of Milled Biomass Part I: Discrete-Particle Models

Feedstock Types

Feedstock Types

- Corn Stover
- Loblolly Pine

Product Types

Product Types

- Diesel Blendstock
- Gasoline Blendstock

Technology Pathways

Technology Pathway

- Direct Liquefaction & Upgrading of Dry Feedstock
- Low Temperature Conversion & Upgrading of Dry Feedstock

Process Area

Process Area

- Conversion
- Preprocessing

Relevant Unit Operations

Unit Operations

- Hopper Feeding
- Pyrolyzer Feed Screw
- Screw Conveyor

QbD Process Parameters

QbD Process Parameter

- Feed Rate

QbD Process Stream Properties

QbD Process Stream Property

- Bulk Density

Multiscale bulk flow characterization

Developed relationships between material attributes and resulting shear and bulk flow properties.

Current Knowledge Gap

- Current state-of-the-art particle mechanics and granular flow models were developed in soil mechanics with test methods appropriate for incompressible, regular solids.
- These test methods do not directly extract equivalent properties for biomass because of the complex interactions of biomass anisotropic compressibility, bulk creep, surface properties and morphology, and heterogeneity/variability.
- Current quasi-static test methods and properties do not directly predict or indicate flow performance in pilot equipment such as has been developed for powders and soils.

Achievement

- Develop multiscale characterization methods and pair with flow validation data to correlate material attributes with bulk flow performance, and lab-scale flow inception and critical state shear properties.

Relevance

- Understanding how characterization methods and material properties impact flow performance will allow for better materials characterization by academia and industrial stakeholders, as well as more robust testing and equipment design for broad bioenergy feedstock.

Task 3 – Material Handling

ACS Sustainable Chemistry & Engineering

Research Article

Impacts of Inorganic Material (Total Ash) on Surface Energy, Wettability, and Cohesion of Corn Stover

Juan H. Leal,* Estrella L. Torres, William Travis Rouse, Cameron M. Moore, Andrew D. Sutton, Amber N. Hoover, Chenlin Li, Michael G. Resch, Bryon S. Donohoe, Allison E. Ray, and Troy A. Semelsberger*

Cite This: ACS Sustainable Chem. Eng. 2020, 8, 2061–2072

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ABSTRACT: The impacts and variability of inorganic material (measured as total ash) on surface area, surface energy, wettability, and cohesion of corn stover samples from Iowa were examined. The impact of total ash on the acid component of surface energy was determined to be significant with the acid component increasing with increasing ash content, in particular, the samples with total ash contents greater than 10%. Negligible effects with ash content were observed on both the dispersive and base components of surface energy. The work of cohesion for the compositions of corn stover with varying amounts of total inorganic matter increased with increasing total ash content, giving rise to potential bulk solids handling and transport challenges related to segregation, agglomeration, rat-holing, arching, and discontinuous flow patterns. Both the wettability (hydrophilicity) and work of cohesion increased for compositions of corn stover with increasing total inorganic content. Washing proved effective at removing extrinsic inorganic material from corn stover with a reduction in total ash content from 20.4% to 6.2%, accompanied by a significant reduction (from 85.6 to 42.5 mJ/m²) in the acid component of the surface energy.

KEYWORDS: Surface energy, Corn stover, Ash, Surface area, Wettability

4 – Progress: Subtask Data Access and Export



- Harmonized, integrated datasets supporting FCIC publications may be easily found, filtered, sorted, and downloaded to Excel or to TSV or CSV text files.
- The integrated LANL, NREL and INL dataset shown below highlights how the Data Hub enables self-service access to the past work of others to supply **Interoperable** and **Reusable** FCIC data in accordance with FAIR data principles.

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KEYWORDS: Surface energy, Corn stover, Ash, Surface area, Wettability

FCIC publication accessible on Web

Data exported to Excel

FCIC Task Portals Studies

Overview Datasets Data Views Results Narratives Workbooks Samples Files Manage

Corn Stover N2 Surface Area and Compositional Analysis

03.05.P1 Bulk Flow Characterization

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Excel Text Script

☒ Excel Workbook (.xlsx) Maximum 1,048,576 rows and 16,384 columns.

☐ Excel Old Binary Workbook (.xls) Maximum 65,536 rows and 256 columns.

☐ Refreshable Web Query (.iqy)

Column headers: Caption

Export

Experiment Name	Composition	Sample ID	Sample INL GUID	Ash Class	Moisture Class	LANL GUID	Average N2 Surface Area M2 G	Assay Date	NREL GUID	Ash wt%	TX ug/g	Al2O3 wt%	Ca O wt%	Fe2O3 wt%	K2O wt%	Mg O wt%	Mn O wt%	Na2O wt%	P2O5 wt%	Si O2 wt%	Ti O2 wt%	SO3 wt%
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment1	ca03f467-348d-e944-94c4-9b4dff2cc3fc	LA	LM	ca03f467-348d-e944-94c4-9b4dff2cc3fc	0.883	2019-05-23	61d60b5d-87ad-804e-b9e3-59acfc2e5a62	7.95	1720.0	5.49	6.04	1.79	10.66	3.58	0.06	0.79	2.49	64.82	0.26	1.35	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment4	fa8f3731-0154-1b41-8f89-b4b20808bc93	LA	LM	fa8f3731-0154-1b41-8f89-b4b20808bc93	0.746	2019-05-23	61f4e57e-ece4-5848-a0b4-10f86f7e698d	8.94	1750.0	6.32	5.92	1.99	8.94	3.27	0.08	0.99	2.56	65.8	0.28	1.31	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment6	f2772330-12f2-bc40-a6d0-218d1051bb4e	LA	LM	f2772330-12f2-bc40-a6d0-218d1051bb4e	0.732	2019-05-23	dcbbc9a4-525d-294d-a85d-aa0c5a018536	8.07	1730.0	5.57	6.09	1.71	11.09	3.22	0.06	0.91	2.74	67.17	0.25	1.38	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale12_Segment2	4c383541-55dc-2441-91e0-a79f5a6c9060	LA	LM	4c383541-55dc-2441-91e0-a79f5a6c9060	0.842	2019-05-23	372bf554-61f1-d742-bc74-8c85daba5cdf	9.48	1630.0	6.58	5.41	2.02	9.5	3.0	0.08	1.08	2.37	68.18	0.29	1.26	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale12_Segment3	cfe01cb9-8d28-f34c-8987-970c4aafc541	LA	LM	cfe01cb9-8d28-f34c-8987-970c4aafc541	0.667	2019-05-23	ad54c824-1ee6-5642-8981-6aec8b8db566a	5.57	1170.0	5.07	7.52	1.61	13.22	4.4	0.07	0.78	3.41	59.12	0.23	1.62	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale12_Segment4	1c2a8dcf-1ea4-a448-8a9b-591589f2502d	LA	LM	1c2a8dcf-1ea4-a448-8a9b-591589f2502d	0.772	2019-05-23	4fa560ea-b90d-da4f-a5ab-077afca7d535	6.73	1490.0	5.29	6.9	1.77	12.93	3.71	0.08	0.78	3.56	61.55	0.26	1.62	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale12_Segment5	cb28b1a0-8251-cf4e-8188-caf0ba6fee5b	LA	LM	cb28b1a0-8251-cf4e-8188-caf0ba6fee5b	0.79	2019-05-23	7a885eba-e618-6d41-a56c-ad8036844c37	9.21	1690.0	6.18	5.65	1.94	9.46	3.02	0.07	0.91	3.01	66.39	0.29	1.33	
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale12_Segment6	49d5d3a1-798b-3f4c-9dbb-39733790aa59	LA	LM	49d5d3a1-798b-3f4c-9dbb-39733790aa59	0.839	2019-05-23	b89f5cf9-0bde-044e-9241-9ae552c936a7	8.04	1470.0	6.03	6.0	1.99	10.9	3.16	0.08	0.84	3.14	65.31	0.3	1.47	

4 – Progress: Data Hub Analytical Tools



Data Analysis: The Task 4 Team is developing reusable data analysis and automated data processing tools using LabKey’s extensive Application Programming Interfaces (APIs) for JMP/SAS, R, Python, Perl, Java, and JavaScript.

Excel

Text

Script

☐ Java

☐ JavaScript

☐ Perl

☐ Python

☒ R

☐ SAS

☐ Stable URL

Create Script

Experiment Name	Composition Sample ID	Sample INL GUID	Ash Class	Moisture Class	LANL GUID	Average N2 Surface Area M2 G	Assay Date	NREL GUID	Ash wt%	TX ug/g	Al2O3 wt%	Ca O wt%	Fe2O3 wt%	K2O wt%	Mg O wt%	Mn O wt%	Na2O wt%	P2O5 wt%	Si O2 wt%	Ti O2 wt%	SO3 wt%
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment1	ca03f467-348d-e944-94c4-9b4dff2cc3fc	LA	LM	ca03f467-348d-e944-94c4-9b4dff2cc3fc	0.883	2019-05-23	61d60b5d-87ad-804e-b9e3-59acfc2e5a62	7.95	1720.0	5.49	6.04	1.79	10.66	3.58	0.06	0.79	2.49	64.82	0.26	1.35
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment4	fa8f3731-0154-1b41-8f89-b4b20808bc93	LA	LM	fa8f3731-0154-1b41-8f89-b4b20808bc93	0.746	2019-05-23	61f4e57e-ece4-5848-a0b4-10f86f7e698d	8.94	1750.0	6.32	5.92	1.99	8.94	3.27	0.08	0.99	2.56	65.8	0.28	1.31
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder	LMLA_Bale11_Segment6	f2772330-12f2-bc40-a6d0-218d1051bb4e	LA	LM	f2772330-12f2-bc40-a6d0-218d1051bb4e	0.732	2019-05-23	dcbb9ca4-525d-a85d-aa0c5a01													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder		4c383541-55dc-2441-91e0-			4c383541-55dc-2441-91e0-	0.842	2019-05-23	372bf554-6f1f-c8c85daba5cdf													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.667	2019-05-23	ad54c824-1ee6-8981-6aec8bdb													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.772	2019-05-23	4fa560ea-b90d-077afca7d535													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.79	2019-05-23	7a885eba-e618-a56c-ad803684													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.839	2019-05-23	b89f5cf9-0bde-49ae552c936a7													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.883	2019-05-23	68f92795-47e7-3bfd3106c9b5													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.775	2019-05-23	4d8a2784-f083-96a3b55e94ca													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						1.007	2019-05-23	7935cc6d-dbe3-9751-98e6f706													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.906	2019-05-23	5d171032-9598-a1b5-e55964b5													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						0.806	2019-05-23	5a387168-e756-bc23-d447c614													
LT Baseline Ash Speciation Analysis After 2nd Stage Grinder						1.052	2019-05-23	ab41b9d9-449b-dff2c1b29da6													

fcic Bioenergy Data Hub

FCIC Task Portals Studies Overview Datasets Data Viewers Results Narratives Workbooks Samples Files Manage

N2 Surface Area vs. Composition

Report Source Help

SVG output

N2 Surface Area vs. Composition

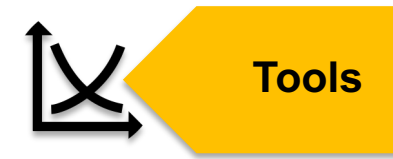
Report Source Help

Script Source

```
1 library(Rlabkey);
2
3 # ${tsvout:tsvfile}
4 labkey.data <- labkey.selectRows(
5   baseUrl="https://bioenergy.labworks.org/labkey",
6   folderPath="/FCIC/FCIC Task Work/T.03.00 Materials Handling/T.03.05.P1 Bulk Flow Characterization",
7   schemaName="study",
8   queryName="Surface_Composition_Join_GUID_Match",
9   viewName="",
10  colSelect="SubjectID,Ash_Class,Moisture_Class,Sample_Description,Average_N2_Surface
11  Area_m2_g,Ash_percent,Composition_Sample_ID,SO3 wt%",
12  colFilter=makeFilter(c("Average_N2_Surface Area_m2_g", "LESS_THAN", "2")),
13  containerFilter=NULL,
14  colNameOpt="fieldname");
15
16 #write.table(labkey.data)
17
18 library(ggplot2);
19 # ${svgout:output.svg}
20 svg("output.svg", width= 18, height=6);
21
22 #ggplot(data = labkey.data, aes(x = (), y = (), label = (Moisture_Class)) + geom_point() +
23   geom_text(size = 3);
24
25 ggplot(data = labkey.data, aes(x = `Average_N2_Surface Area_m2_g`, y = (`SO3 wt%`), label =
26   Moisture_Class)) + geom_point(color= `dodgerblue2`, size = 8) + geom_text(size = 3, color='white') +
27   geom_smooth(method=lm, color= `#2C3E50`) + xlab(bquote("Average Nitrogen Surface Area m2/g")) +
28   ylab(bquote("SO3 wt%"));
```

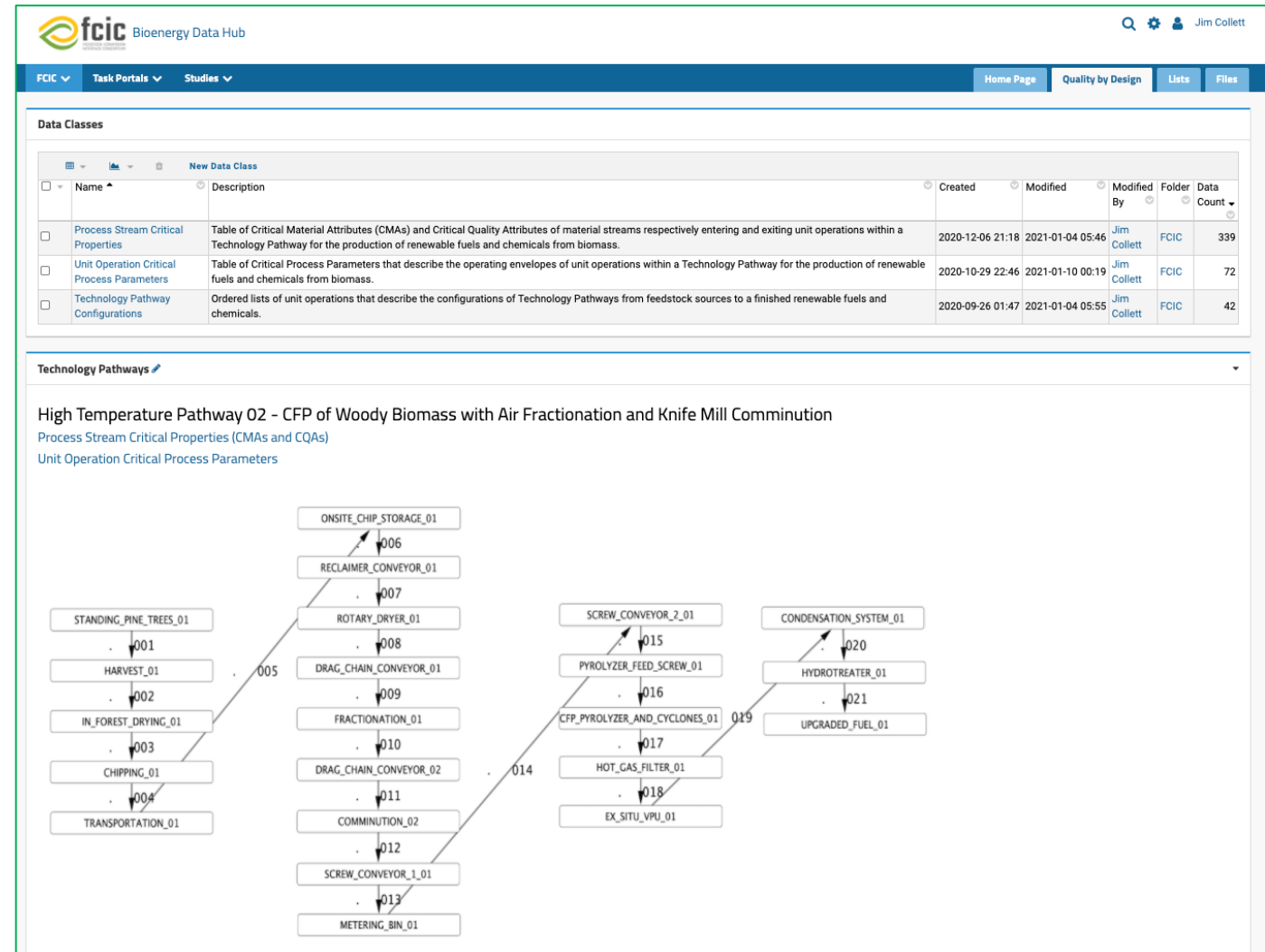
Task 4 – Data Integration 36

4 – Progress: Quality by Design Data Integration

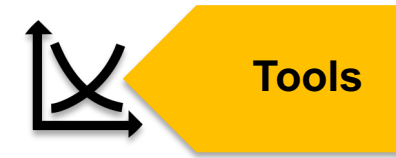


Mapping QbD Properties onto Technology Pathways

- Process Stream Critical Properties
- Unit Operation Critical Process Parameters
- Collaborative QbD property assignment supports:
 - self-organization of metadata into ontologies within the FCIC community.
 - consensus for defining controlled vocabularies and units of measure for use across the growing bioeconomy.



4 – Progress: Quality by Design Data Integration



- A Process Stream Critical Properties data table was created for managing the assignment of QbD critical material properties to feedstocks, intermediates, and products within the High- and Low-Temperature Conversion pathways.
- A related Unit Operation Critical Process Parameters data table was created for assignment of critical process parameters to unit operations within the High- and Low-Temperature Conversion technology pathways.
- Subtask teams and the FCIC PI have reached consensus on a first batch of 164 input material attributes, 85 output quality attributes, and 79 process parameters; these data are now being harmonized and uploaded to the database.

1 - 12 of 12												
default This grid view has been modified. Revert Edit Save												
✖ Material Property IS ONE OF (MOISTU... ✖ Unit Op IS ONE OF (DRAG_CHAIN_CON... Clear All												
<input type="checkbox"/>	Tech Pathway	Unit Op	Intermediate Stream	Intermediate State	Material Property	Units	CMA Upper Limit	CMA Lower Limit	CQA Upper Limit	CQA Lower Limit	Downstream Unit Op	Critical Downstream Unit Op
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	009	Chips	ASH_CONTENT_01	%	30.0	4.0	30.0	4.0	FRACTIONATION_01	COMMINUTION_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	009	Chips	PARTICLE_SIZE_DISTRIBUTION_01	mm	50.0	6.0	50.0	6.0	FRACTIONATION_01	COMMINUTION_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	009	Chips	MOISTURE_CONTENT_01	%	35.0	10.0	35.0	10.0	FRACTIONATION_01	COMMINUTION_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	FRACTIONATION_01	010	Chips	PARTICLE_SIZE_DISTRIBUTION_01	mm					DRAG_CHAIN_CONVEYOR_01	
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	FRACTIONATION_01	010	Chips	ASH_CONTENT_01	%					DRAG_CHAIN_CONVEYOR_01	
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	FRACTIONATION_01	010	Chips	MOISTURE_CONTENT_01	%					DRAG_CHAIN_CONVEYOR_01	
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	011	Chips	PARTICLE_SIZE_DISTRIBUTION_01	mm	50.0	6.0		1.0	COMMINUTION_02	PYROLYZER_FEED_SCREW_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	011	Chips	ASH_CONTENT_01	%	30.0	4.0		0.0	COMMINUTION_02	PYROLYZER_FEED_SCREW_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	DRAG_CHAIN_CONVEYOR_01	011	Chips	MOISTURE_CONTENT_01	%	35.0	10.0		3.0	COMMINUTION_02	PYROLYZER_FEED_SCREW_01
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	COMMINUTION_02	012	Particles	PARTICLE_SIZE_DISTRIBUTION_01	mm					SCREW_CONVEYOR_1_01	
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	COMMINUTION_02	012	Particles	ASH_CONTENT_01	%					SCREW_CONVEYOR_1_01	
<input type="checkbox"/>	HIGH_TEMPERATURE_CONVERSION_02	COMMINUTION_02	012	Particles	MOISTURE_CONTENT_01	%					SCREW_CONVEYOR_1_01	



Data shown are not actual and are provided for layout demonstration only

4 – Progress: Access to Data for QbD Critical Property Assignment



- The QbD tables support links to experimental data that may be considered in the assignment of sets of critical properties to process intermediate streams or unit operations.

Unit Op IS ONE

Lists / Material Quality Classes

View List Item FCIC

Material or Quality Attribute: ASH_CONTENT_01

Data Type: Scalar

Units: %

Parent Assay: Ash Percent 750C

Description:

Area Unit Op Equipment Type Material Property Parent Assay CMA Upper Limit CMA Lower Limit Intermediate Stream Number CQA Upper Limit CQA Lower Limit Downstream Unit Op

ESSING ROTARY_DRYER_01 Dryer ASH_CONTENT_01 Ash Content 750C ASTM D3174-12 30.0 4.0 008 30.0 4.0 DRAG_CHAIN_CONVEYOR_01

ESSING ROTARY_DRYER_01 Dryer MOISTURE_CONTENT_01 Moisture (% 105C) 60.0 10.0 008 35.0 10.0 DRAG_CHAIN_CONVEYOR_01

ESSING ROTARY_DRYER_01 Dryer PARTICLE_SIZE_DISTRIBUTION_01 Particle Size Distribution-Forage Separator 50.0 6.0 008 50.0 6.0 DRAG_CHAIN_CONVEYOR_01

ESSING COMMINATION_01 Hammer Mill ASH_CONTENT_01 Ash Content 750C ASTM D3174-12 30.0 4.0 010a 3.0 0.0 SCREW_CONVEYOR_1_01

ESSING COMMINATION_01 Hammer Mill MOISTURE_CONTENT_01 Moisture (% 105C) 35.0 10.0 010a 15.0 3.0 SCREW_CONVEYOR_1_01

ESSING COMMINATION_01 Hammer Mill PARTICLE_SIZE_DISTRIBUTION_01 Particle Size Distribution-Forage Separator 50.0 6.0 010a 6.0 1.0 SCREW_CONVEYOR_1_01

20,21 1,5 HIGH_TEMPERATURE_CONVERSION_01 PREPROCESSING COMMINATION_02 Knife Mill ASH_CONTENT_01 Ash Content 750C ASTM D3174-12 010b SCREW_CONVEYOR_1_01

20,21 1,5 HIGH_TEMPERATURE_CONVERSION_01 PREPROCESSING COMMINATION_02 Knife Mill MOISTURE_CONTENT_01 Moisture (% 105C) SCREW_CONVEYOR_1_01

PARTICLE_SIZE_DISTRIBUTION_01 Particle Size Distribution-Forage Separator SCREW_CONVEYOR_1_01

ASH_CONTENT_01 Ash Content 750C ASTM D3174-12 METERING_BIN_01

MOISTURE_CONTENT_01 Moisture (% 105C) METERING_BIN_01

PARTICLE_SIZE_DISTRIBUTION_01 Particle Size Distribution-Forage Separator METERING_BIN_01

ASH_CONTENT_01 Ash Content 750C ASTM D3174-12 SCREW_CONVEYOR_2_01

MOISTURE_CONTENT_01 Moisture (% 105C) SCREW_CONVEYOR_2_01

PARTICLE_SIZE_DISTRIBUTION_01 Particle Size Distribution-Forage Separator SCREW_CONVEYOR_2_01

Assay List / Ash (% 750C) Batches / Ash (% 750C) Runs

Ash (% 750C) Results FCIC

Dry-basis %ash measured from TGA based on ASTM D 3172-07.

MANAGE ASSAY DESIGN VIEW BATCHES VIEW RUNS VIEW RESULTS VIEW COPY-TO-STUDY HISTORY VIEW EXCLUDED DATA

Copy To Study Import Data Re-import Run Replaced Filter Exclude 1 - 7 of 7

default This grid view has been modified. Revert Edit Save

Run = 685

Experiment Name Sample ID BFL GUID Date Ash Percent 750C Protocol Wiki Page

HT Baseline Analysis Dry2-HAHM-D6 04a76489-db6b-da43-a60f-912accd96bef 2018-07-10 00:00 1.1874 Ash Percentage 750C

HT Baseline Analysis Dry2-LAHM-D19 5c29330f-03b5-d447-80ae-fc47feb0c504 2018-07-10 00:00 0.5096 Ash Percentage 750C

HT Baseline Analysis Dry2-LAHM-D3 f200d4c5-9afb-d94c-9d85-3c90dab93c41 2018-07-10 00:00 0.3731 Ash Percentage 750C

HT Baseline Analysis Stg2-HALM-C4 c6309fbc-6cdc-1e45-8ac7-b943b5d7060a 2018-07-10 00:00 4.1305 Ash Percentage 750C

HT Baseline Analysis Stg2-HALM-C7 f5f70c25-6f66-1d48-aed9-1dc4195a9206 2018-07-10 00:00 2.8119 Ash Percentage 750C

HT Baseline Analysis Stg2-LALM-C4 550e0857-f909-d147-9a76-a6fee1f3315a 2018-07-10 00:00 0.7436 Ash Percentage 750C

HT Baseline Analysis Stg2-LALM-C6 7599e95e-a198-8b48-af95-deb1b4021315 2018-07-10 00:00 0.6984 Ash Percentage 750C

Start Page / Assay Management

Ash Percentage 750C FCIC

Edit New Manage

Designation: D3174 - 12

Standard Test Method for Ash in the Analysis Sample of Coal and Coke from Coal¹

This standard is issued under the third designation D3174, the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last revision or superseding edition (s) indicates an editorial change since the last revision or reapproval.

This standard has been approved for use by agencies of the U.S. Department of Defense.

1. Scope

1.1 This test method covers the determination of the inorganic residue as ash in the analysis sample of coal or coke as prepared in accordance with Practice D2013 or Practice D346. The results obtained can be applied as the ash in the proximate analysis, Practice D3172, and in the ultimate analysis, Practice D3176. For the determination of the constituents in ash, reference is made to Test Methods D3682, D4326 and D6349. Test Method D6357 should be used to prepare ash to be used for trace element analysis. See Terminology D121 for definition of ash.

1.2 The values stated in SI units are to be regarded as

D3172 Practice for Proximate Analysis of Coal and Coke

D3173 Test Method for Moisture in the Analysis Sample of Coal and Coke

D3176 Practice for Ultimate Analysis of Coal and Coke

D3180 Practice for Calculating Coal and Coke Analyses from As-Determined to Different Bases

D3682 Test Method for Major and Minor Elements in Combustion Residues from Coal Utilization Processes

D4326 Test Method for Major and Minor Elements in Coal and Coke Ash By X-Ray Fluorescence

D5016 Test Method for Total Sulfur in Coal and Coke

Combustion Residues Using a High-Temperature Tube Furnace Combustion Method with Infrared Absorption

Data shown are not actual and are provided for layout demonstration only

Task 4 – Data Integration 39

4 – Progress: Experimental Data Integration



- Screenshot shows part of a dataset containing 216 records with 224 data columns integrated via a simple SQL query from 3 uploaded data files containing:

- Feedstock property data from INL
- Bio-oil property data and pyrolyzer run metadata from NREL
- Fuel property data and hydrotreater run metadata from PNNL

- Stable, reusable SQL code and user access to source files promotes trust in large datasets on the Data Hub for data mining analysis and machine learning.
- Performing such integrations manually in Excel is time-consuming and error-prone.

fcic

Bioenergy Data Hub

Jim Collett

FCIC

Task Portals

Studies

Overview

Subjects

Data Views

Manage

FP and HT Joined Data 1 - Selected Fields

Pyrolysis Bio-Oil and Hydrotreater Data Integration

PR 2021

Py Feed Type IS ONE OF (air classified ...)

INL Feedstock GUID	Py Feed Type	HT Feed Type	Py FP Run Or Oil ID	HT Feed Provider Run Number	PNNL HT Run Number	Py Run Date	HT Run Date	Py Pyrolyzer ID	HT Provider Reactor Type	HT HT Reactor	Py FP Total Liquids Wt Pct	HT Upgraded Oil Yield g/g	Py Char Yield Pct	Py Gas Yield Pct	HT Gasoline Fraction Wt Pct	HT Diesel Fraction Wt Pct	HT Jet Fuel Fraction Wt Pct	HT Heavies Fraction Wt Pct	Py Carbon Wt Pct	HT C Wt Pct	Py Hydrogen Wt Pct	HT H Wt Pct	Py Nitrogen Wt Pct	HT N Wt Pct	Py Oxygen Wt Pct	HT O Wt Pct	Py S Wt Pct	HT S Wt Pct	Py Water Wt Pct	HT Viscosity C P 40C	HT Gas Yield g/g	HT Carbon Balance g/g	HT Mass Balance g/g
032b4e7c-2d86-434b-9aec-3fa7980e2e1e	Loblolly Pine (whole pine)	whole pine (LWP)	6116-037	6116-037	62006-3	1776-01-02 15:00	2015-05-19 00:00	2FBR	2FBR	PDLE	65.7	0.462	13.4	15.8	38.7412	43.8466	28.3682	17.4123	46.1	88.09	7.5	12.6	0.07	0.0	46.2	1.03	51.1159	0.0	20.5	1.056	0.163	0.8723	0.9361
17113d89-e706-ae4d-9548-b0950fac5ae9	Whole Pine (WP)	Whole Pine	5858-021	5858-021	61573-43	1776-01-02 15:00	2014-06-19 00:00	2FBR	2FBR	PDLE	62.9	0.501	15.0	18.9	42.0	44.0	11.0	14.0	45.3	87.52	8.1	12.67	0.09	0.0	46.5	1.03	41.0	0.0	22.5	1.0545	0.141	0.8763	0.998
3138a563-ace0-eb46-8658-0a209687545e	Tulip Poplar (TP)	Tulip Poplar Repeat	5858-074	5858-074	61573-51	1776-01-02 15:00	2014-07-31 00:00	2FBR	2FBR	PDLE	70.6	0.401	7.6	13.5	40.0	46.0	12.0	14.0	44.8	86.05	7.7	11.99	0.08	0.0	47.4	0.69	48.0	0.0	18.8	1.2003	0.191	0.8368	0.955
427efecf-f5a2-974c-b19a-5918a53ec5d2	Hybrid Poplar (HP)	Hybrid Poplar	5858-020	5858-020	61573-45	1776-01-02 15:00	2014-06-26 00:00	2FBR	2FBR	PDLE	64.9	0.46	8.9	19.2	45.0	42.0	11.0	13.0	45.9	86.76	8.1	12.42	0.08	0.0	45.9	1.01	56.0	0.0	20.7	0.9677	0.172	0.8821	1.001
88e73d0e-9e8d-a842-8c41-4e8125a90dc7	Loblolly Pine (CP)	Clean Pine	5858-023	5858-023	61573-42	1776-01-02 15:00	2014-06-19 00:00	2FBR	2FBR	PDLE	65.2	0.515	12.0	17.9	39.0	44.0	12.0	17.0	45.0	87.15	7.8	12.516	0.08	0.0	47.1	1.082	37.0	0.0	21.1	1.2186	0.152	0.9275	1.015
972be12c-a954-624f-955f-735c83a95f2d	Loblolly Pine (CP)	Loblolly pine	6408-001	6408-001	62006-42	1776-01-02 15:00	2016-08-02 00:00	2FBR	2FBR	PDLE	70.7	0.443	10.5	13.6	43.8531	29.0193	9.2955	88.6177	46.59	88.24	7.08	12.58	0.04	0.0	46.3	0.728	49.0	0.007	18.1	1.1916	0.22	0.911	0.994
977176f3-92e4-cb40-ad2d-0b217c3aa061	Loblolly Pine (clean pine)	clean pine (LPC)	6116-020	6116-020	61573-72	1776-01-02 15:00	2015-03-02 00:00	2FBR	2FBR	PDLE	63.1	0.481	12.3	17.7	41.4432	45.0307	29.7181	13.5261	47.0	87.82	7.5	12.82	0.06	0.0	44.9	1.09	51.2521	0.02	21.7	0.945	0.191	0.914	0.994
cec77c74-4ce7-734a-bd28-9d14ec81530c	Forest Residue (FR)	Forest Residue	6207-102	6207-102	62005-40	1776-01-02 15:00	2016-06-07 00:00	2FBR	2FBR	PDLE	62.0	0.466	19.1	16.5	46.5527	42.9406	29.111	10.5067	40.19	88.63	7.87	12.38	0.19	0.0	51.75	1.044	158.0	0.016	16.4	1.2532	0.156	1.045	1.0
df5ebbcc-b8de-ba48-8cc7-c245af6b5b35	air classified Forest Residue (acFR)	air cleaned FR	6408-080	6408-080	62006-48	1776-01-02 15:00	2016-09-16 00:00	2FBR	2FBR	PDLE	67.5	0.491	13.1	14.8	42.9938	28.2799	12.4186	90.4751	48.48	87.97	7.48	12.38	0.03	0.0	44.0	1.0	87.0	0.0079	17.3	1.3633	0.172	0.912	1.0
e717596a-c33b-a745-ae21-85d720d68f6b	Pinion_Juniper	pinion juniper (PJ)	6116-011	6116-011	61573-74	1776-01-02 15:00	2015-03-10 00:00	2FBR	2FBR	PDLE	57.9	0.176	15.3	17.5	60.5703	37.3962	37.0407	2.0336	50.3	86.86	8.6	14.03	0.49	0.0	40.3	1.13	245.7353	0.0	27.6	0.495	0.178	0.3784	0.8978

